Manual for Powder Indexing Software Conograph

Oct 2015

Contents

Acknowledgments

We would like to express our gratitude to the professors of Ibaraki University, Tokyo Institute of Technology, and the High Energy Accelerator Research Organization for providing powder diffraction data for this project. We would also like to thank the staff of the Visible Information Center, Inc. for their cooperation in developing the GUI. This software was developed with the support of the Grant-in-Aid for Young Scientists (B) (No. 22740077) and funding from Ibaraki Prefecture (J-PARC-23D06).

1. Overall configuration

Conograph was developed by the High Energy Accelerator Research Organization for running two command-user-interface (CUI) programs for powder indexing and peak searching through operations on a graphical user interface.

Fig. 1-1 shows a screenshot of the Conograph user interface.

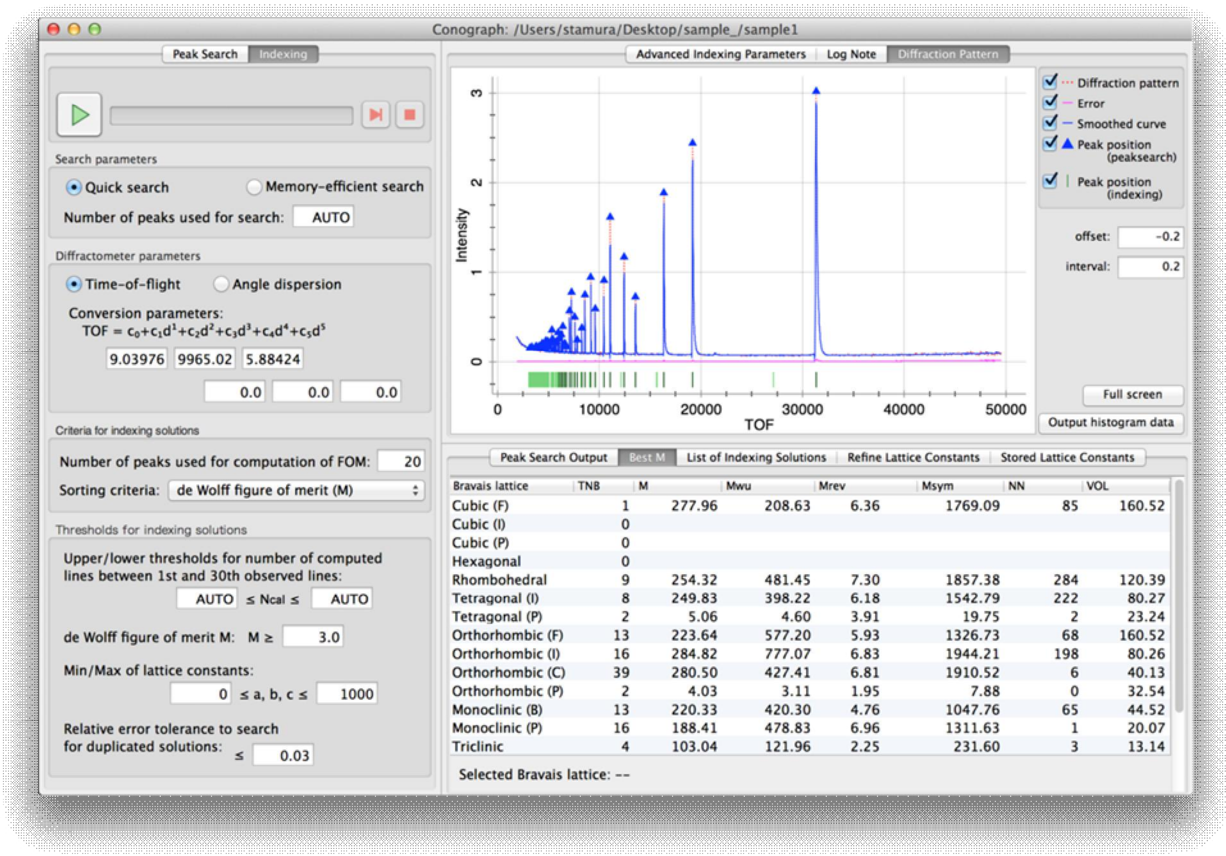


Fig. 1-1 Conograph user interface

2. Creating new project/opening existing project

Fig. 1-1 shows a screenshot of the Conograph UI immediately after the application is started. To conduct peak searches or indexing, it is necessary to create a new project or open an existing project.

This chapter explains the procedures for both operations.

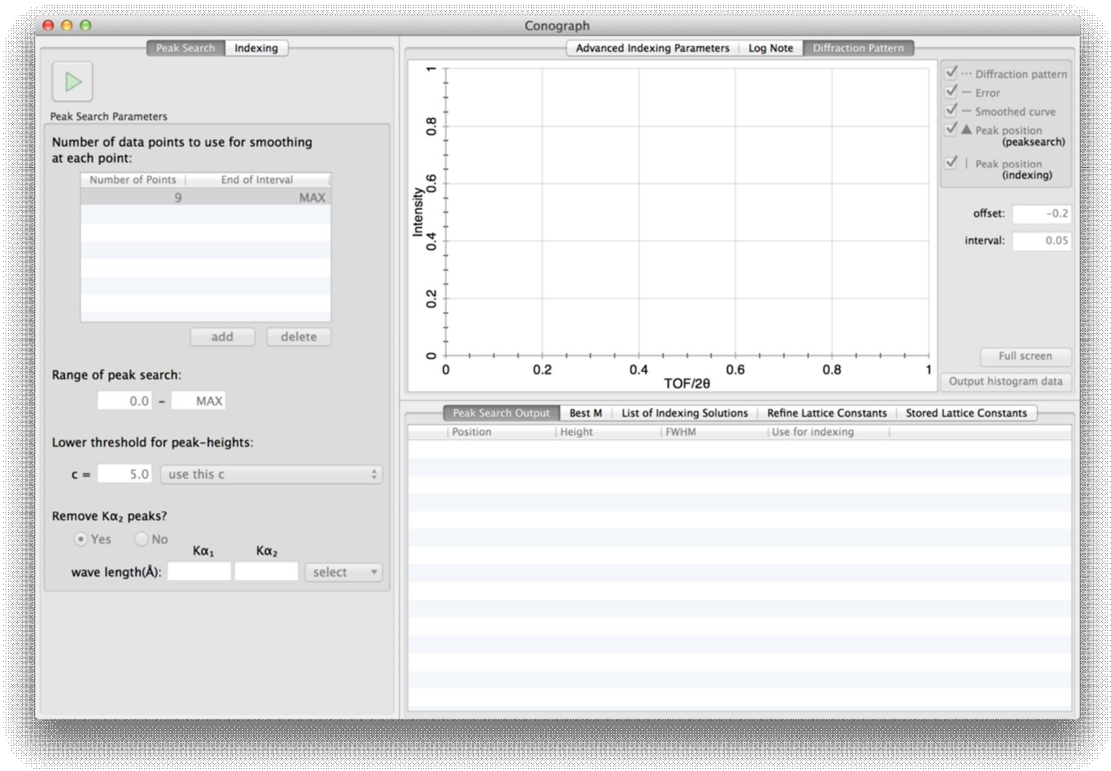
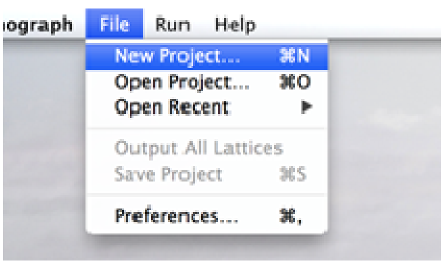


Fig. 2-1 Screenshot immediately after opening Conograph

2.1. Creating a new project

To create a new project, first select **File > New project** as shown below.



In the dialog box for creating projects, you can specify the diffraction data file and project folder, as shown in Fig. 2-2.

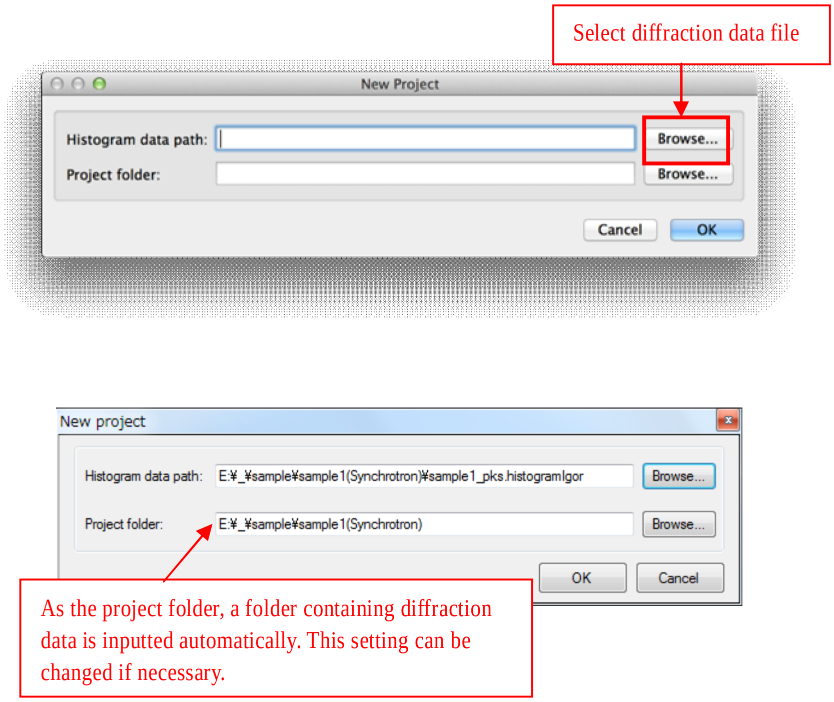
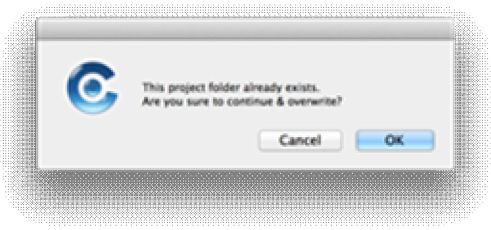


Fig. 2-2 Dialog box for creating new project

The diffraction data file can be formatted in three types of format: XY (Fig. 2-3), IGOR (Fig. 2-4), and Rietan (Fig. 2-5). For the XY and IGOR formats, the observation errors of y-values (in the second column) can be input in the third data column. If the third column is empty, the roots of the y-values are used as the observation errors. In the file, LF, CR+LF, and CR can be used as a line feed code, and spaces and tabs as a delimiter.

The project is created by clicking the OK button after providing the project information. A folder named **auto_generated_files** is created in the project folder, and used to store all the automatically outputted files. This folder contains all the files necessary for using Conograph. Thus, it contains a copy of the diffraction data file specified in Fig. 2-2 and parameter set up files (Fig. 11-1ð).

When the specified project folder already exists and contains the **auto_generated_files** folder as a subfolder, the following dialog box appears:



If you select **Yes**, all the files originally present in the **auto_generated_files** folder are deleted and cannot be retrieved.

```
tof     yint    yerr
7.00000 4942    70.29935988
7.01697 4956    70.39886363
7.03395 5084    71.30217388
～omitted～
89.66605        818     28.60069929
89.68303        818     28.60069929
89.70000        818     28.60069929
```

Fig. 2-3　Example of XY format

```
IGOR
WAVES/O tof, yint, yerr
BEGIN
  8792.00000         0.85962         0.05899
  8808.00000         0.79276         0.05643
  8824.00000         0.75064         0.05470
～omitted～
199536.00000         0.40015         0.01698
199664.00000         0.36920         0.01634
199792.00000         0.39202         0.01686
END
```

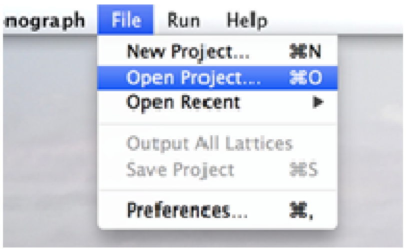
Fig. 2-4　Example of IGOR format

```
3500    10.0000 0.0200
15, 16, 26, 19
30, 15, 23, 22
26, 25, 20, 17
～omitted～
8, 12, 4, 9
13, 12, 8, 6
7, 6, 11, 1
```

Fig. 2-5　Example of Rietan format

2.2. Opening a project

To open an existing project, select **File > Open project** as shown below.



Then, the file folder selection dialog box is displayed. You can specify a project folder in the dialog box.

Fig. 2-3 shows the status of the software immediately after a project is opened and the diffraction pattern file and parameter setup file (***.inp.xml**) are loaded. In the **Diffraction pattern** frame (red square in the figure), the measured diffraction pattern (é) and errors (' , only when there is an error in the diffraction pattern file) are displayed.

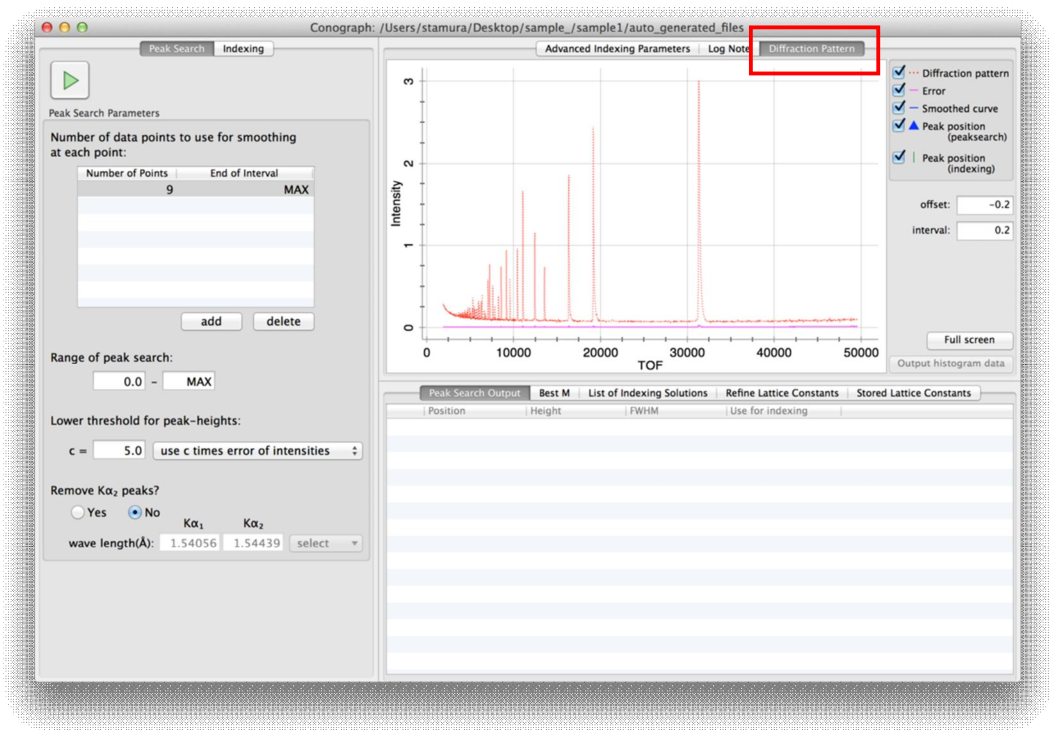


Fig. 2-6 Screenshot immediately after opening a project (prior to peak search)

If a peak search has been performed in the opened project and the file ***_pks.histogramIgor** exists, the indexing frame is displayed, as shown in Fig. 2-7. In addition to the diffraction pattern (é), the peak positions (ƶ) and a smoothed diffraction pattern (') are displayed.

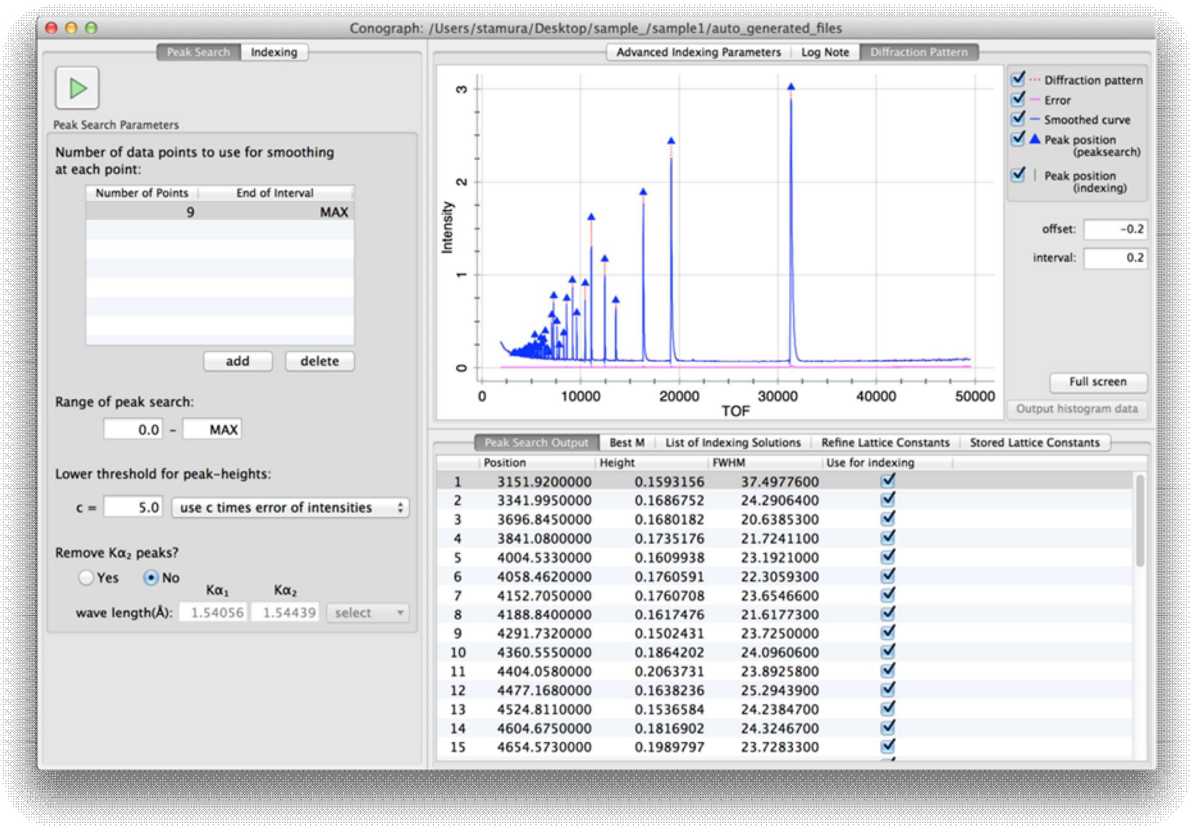


Fig. 2-7 Screenshot immediately after opening a project (after peak search)

Further, when a backup file exists, the project is opened, loading indexing results saved in the backup file.

3. Peak search

3.1. Peak search execution

After opening the project, first, a peak search must be performed in order to obtain peak positions for indexing. A peak search is performed using the **Peak search** frame:

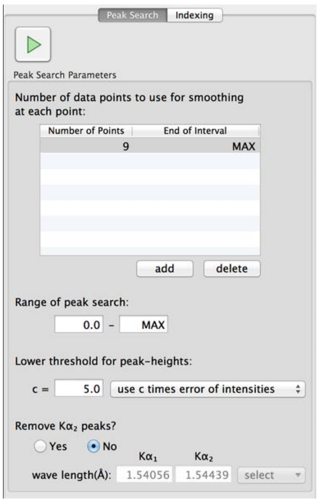


Fig. 3-1 explains the operations available in the **Peak search** frame.

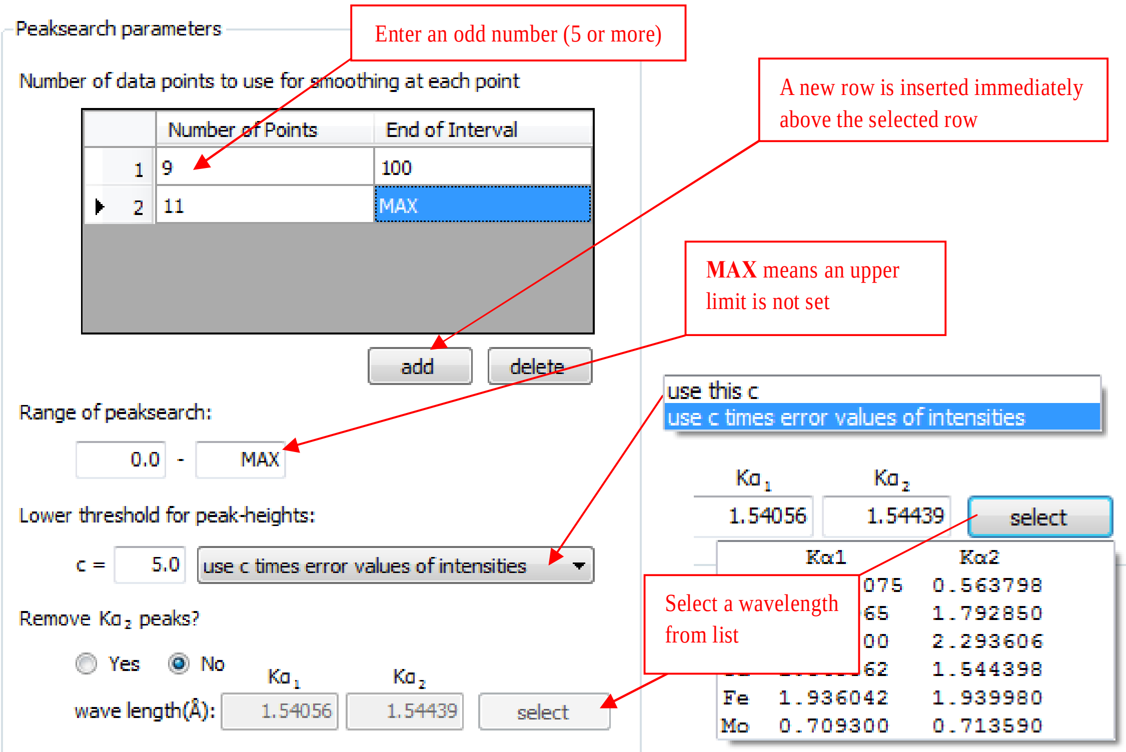
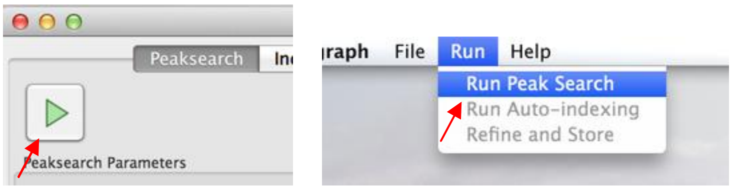
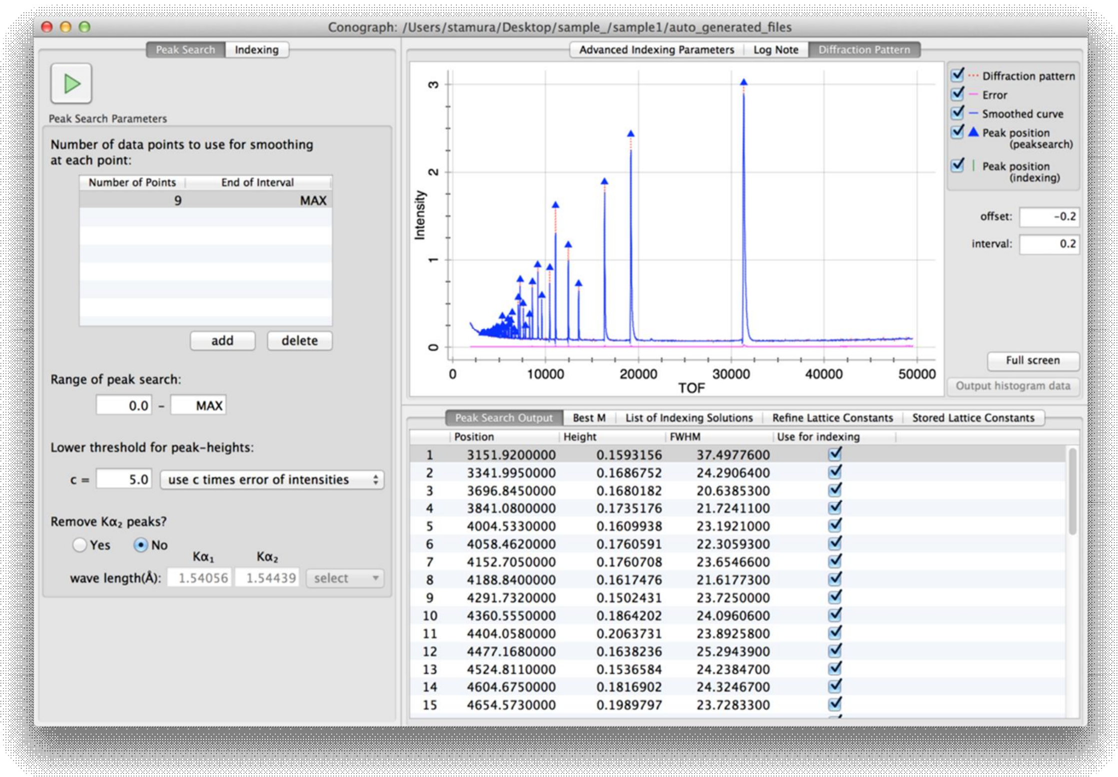


Fig. 3-1 Setting peak search parameters

To conduct a peak search, click the Run button  or select **Menu > Run > Run peak search**:



When the peak search is completed, the screen appears as follows.



In the **Diffraction Pattern** frame, a smoothed diffraction pattern (') and peak positions (z) are displayed. Simultaneously, they are stored in the file **auto_generated_files folder/*_pks.hstogramIgor**[1].

[1]If the peak search results found at the end of the ***_pks.histogramIgor** file (Fig. 11-4) are modified using a text editor, the results are loaded on the application when the same project is reopened.

3.2. Checking peak search results

To obtain appropriate peak search results for indexing, you should check whether the following problems occur, in particular, for the low-angle peaks, by magnifying the graphical display of the diffraction pattern:

- Are there many diffraction peaks that have not been detected?
- Has noise (including small peaks that may not be diffraction peaks) been detected as a peak?

The aforementioned problems during peak search can be resolved by adjusting some of the peak search parameters and re-executing peak search (for parameter adjustment, refer to Section 10.1).

The graph magnification in the **Diffraction Pattern** frame is changed by using the mouse wheel or rubber band (= rectangular range) selection using left drag. A parallel shift of the display area is achieved by using **Ctrl + left drag** or **center drag**. The shortcut menu that appears when you right-click on the graph is shown in Fig. 3-2. Its components and their descriptions are listed in Table 3-1.

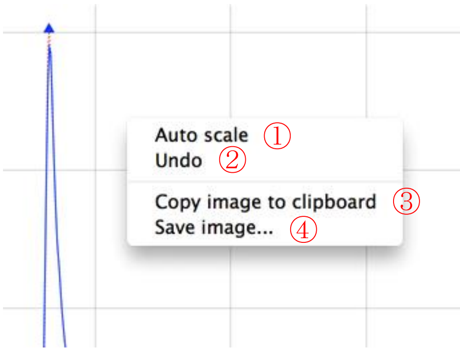


Fig. 3-2 Shortcut menu

Table 3-1 Shortcut menu

①	Adjusts scale to fit entire graph
②	Returns to the previous display status
③	Copies graph contents onto the clipboard
④	Saves graph contents in an image file

3.3. Removing and adding peaks manually

This section introduces a method for modifying peak search results using the GUI operations. However, even if the results are not satisfactory, you should attempt to adjust the peak search parameters first, before proceeding to the following operations.

Peaks used in indexing can be selected using the check boxes that appear in the **Use for indexing** column in the **Peak Search Output** frame (Fig. 3-3). Whether or not peaks are used is represented visually in the **Diffraction Pattern** frame, as shown in Fig. 3-4.

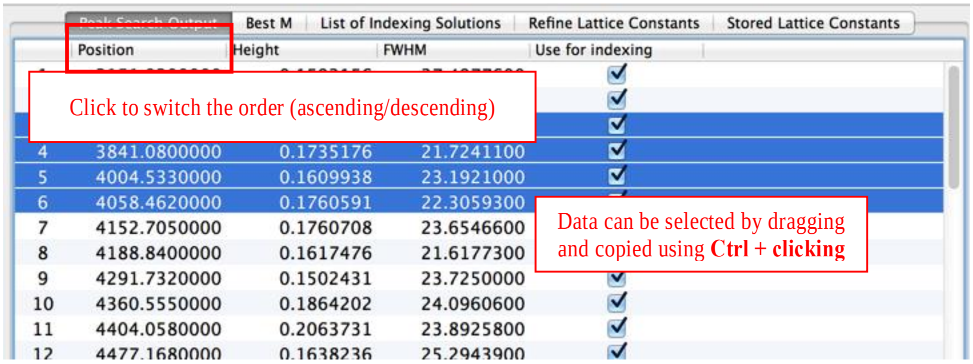


Fig. 3-3 Input peak positions

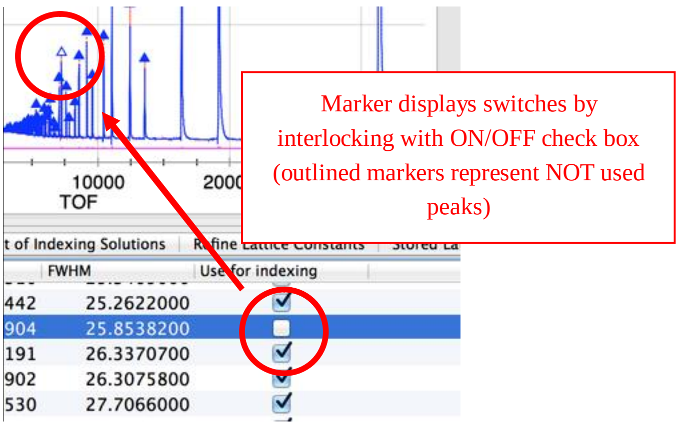


Fig. 3-4 Representation of NOT used peaks in the Diffraction Pattern frame

A peak can be inserted manually at the mouse pointer position by double-clicking on the diffraction pattern. Its height is automatically decided by interpolation. The specific values of the peak position and the full width at half maximum (FWHM) can be edited in the **Peak Search Output** frame (Fig. 3-5).

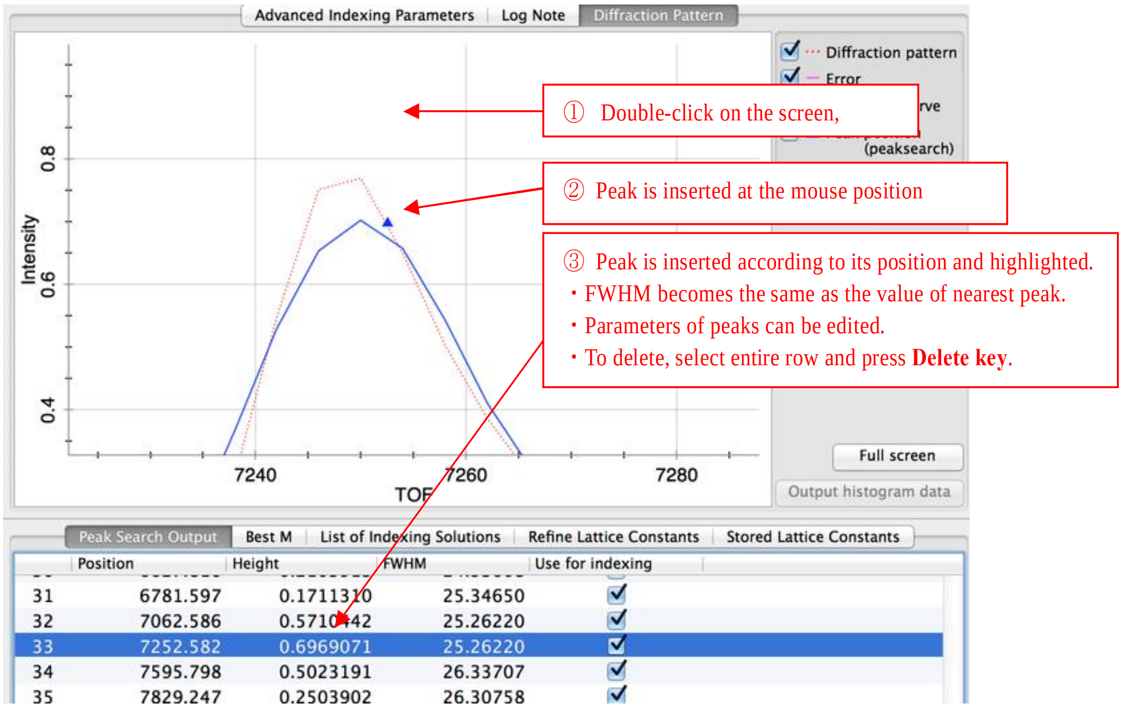


Fig. 3-5 Manual insertion of a peak

4. Parameters used for indexing

The parameters used in indexing are located in three frames (Fig. 4-1):

1. **Indexing** frame
   a. Search parameters and diffractometer parameters
   b. Sorting criteria and thresholds for lattice parameters displayed in the list (can be changed after indexing)
2. **Advanced indexing parameters** frame
3. **Peak Search Output** frame

Immediately after a new project is created, the values recommended for the respective parameters are set. Basically, it is not necessary to change the values, except for the diffractometer parameters.

The parameter in item 3 above is introduced in Section 3.3. The criteria and thresholds in item 1b are introduced in Section 5.3, because they can be changed even after indexing. In the current section, the remaining two types of parameters are explained.

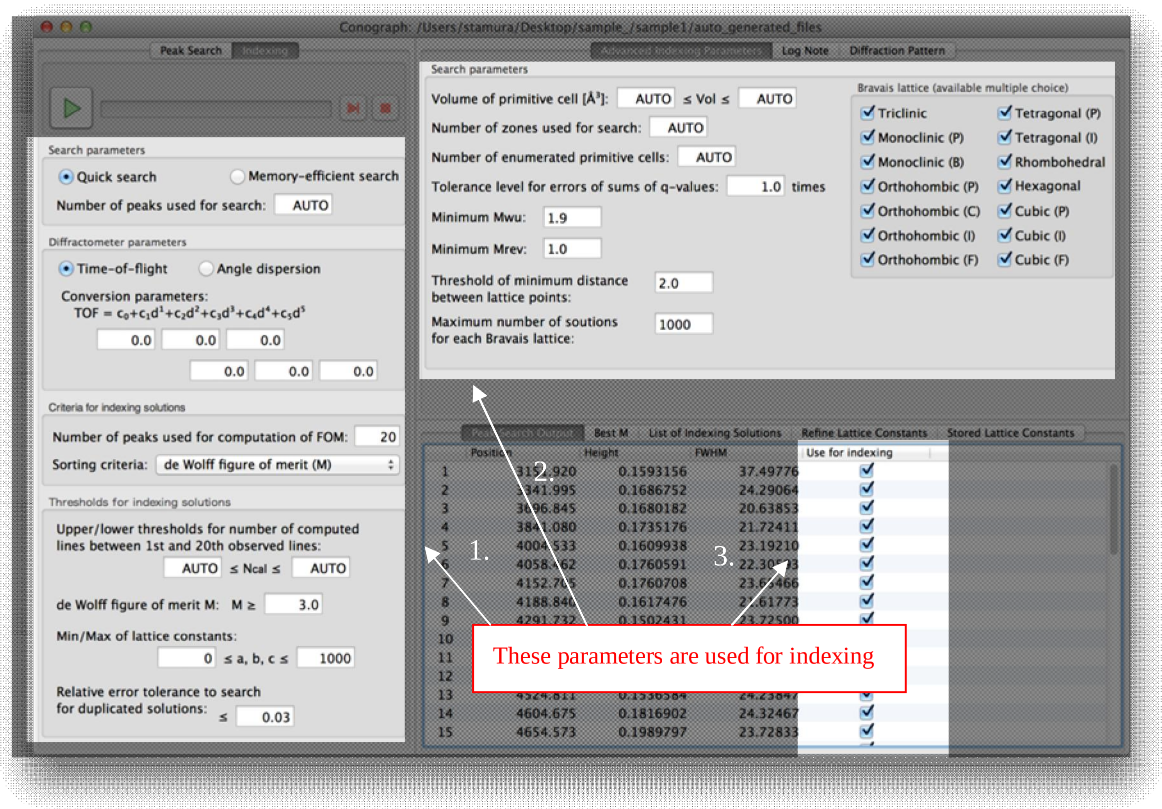


Fig. 4-1 Input parameters of powder indexing

4.1. Search parameters and diffractometer parameters

In the **Search parameters** area, the search method and number of peaks used for powder indexing can be specified. There are two search method options:

- Quick search (when the size of the unit cell is small or for cases with high symmetry),
- Exhaustive search (for all cases)

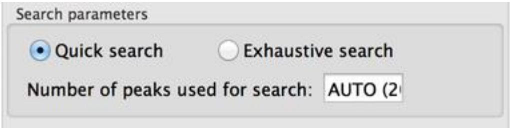


Fig. 4-2 Search parameters

Since the basic algorithms of the two search methods are the same, the two methods can return the same result, if you adjust the parameters used for the quick search.

Powder indexing with **Quick search** is successful in many cases. However, **Memory-efficient search** should be used in more difficult cases. Powder indexing with **Memory-efficient search** occasionally takes more than 10 minutes.

In the **Diffractometer parameters** area, the time-of-flight or angle dispersion method can be selected. Except for the zero point shift, the parameter values are unique to the respective diffractometer (Fig. 4-3, Fig. 4-4, and Table 4-1). Entering 0 deg. for the zero point shift is normally effective. More precise values can be estimated by executing refinement after indexing.

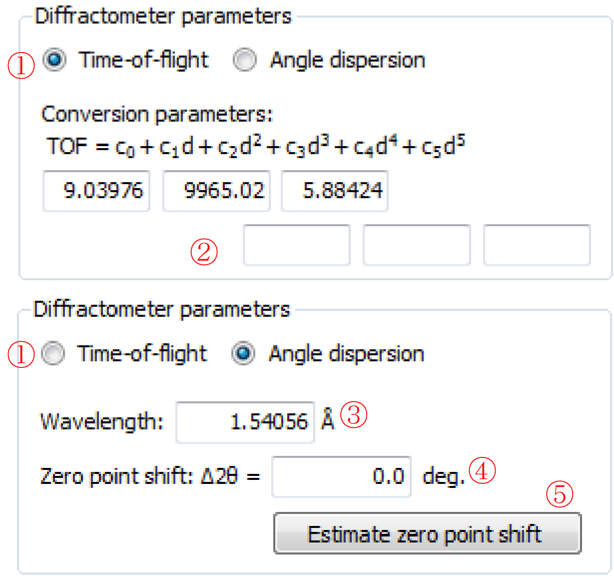


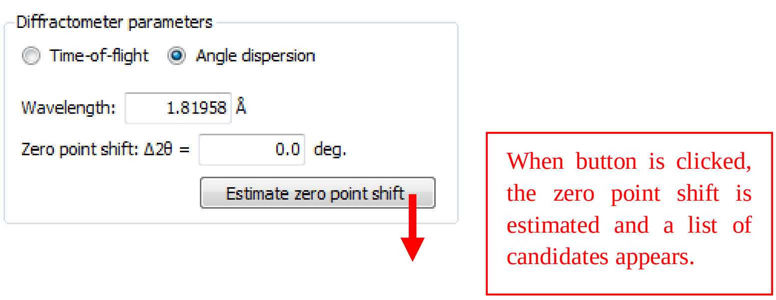
Fig. 4-3 Diffractometer parameters

(Top: Time-of-flight method; Bottom: Angle dispersion method)

Table 4-1 Diffractometer parameters

①	Selects ñTime-of-flightò or ñAngle dispersionò
②	Conversion parameters represented as polynomial coefficients from zero to fifth order
③	Wavelength [Å]
④	Peak shift parameter æ2θ [degrees]
⑤	Estimates zero point shift by using the reflection pair method

The zero point shift can be estimated by conducting the reflection pair method [1] (Fig. 4-3). In the reflection point method, the zero point shift is estimated by using two peak positions that have a ratio of d-values equal to two-fold. As shown in Fig. 4-3, the one that appears to be correct can be selected from various candidates.



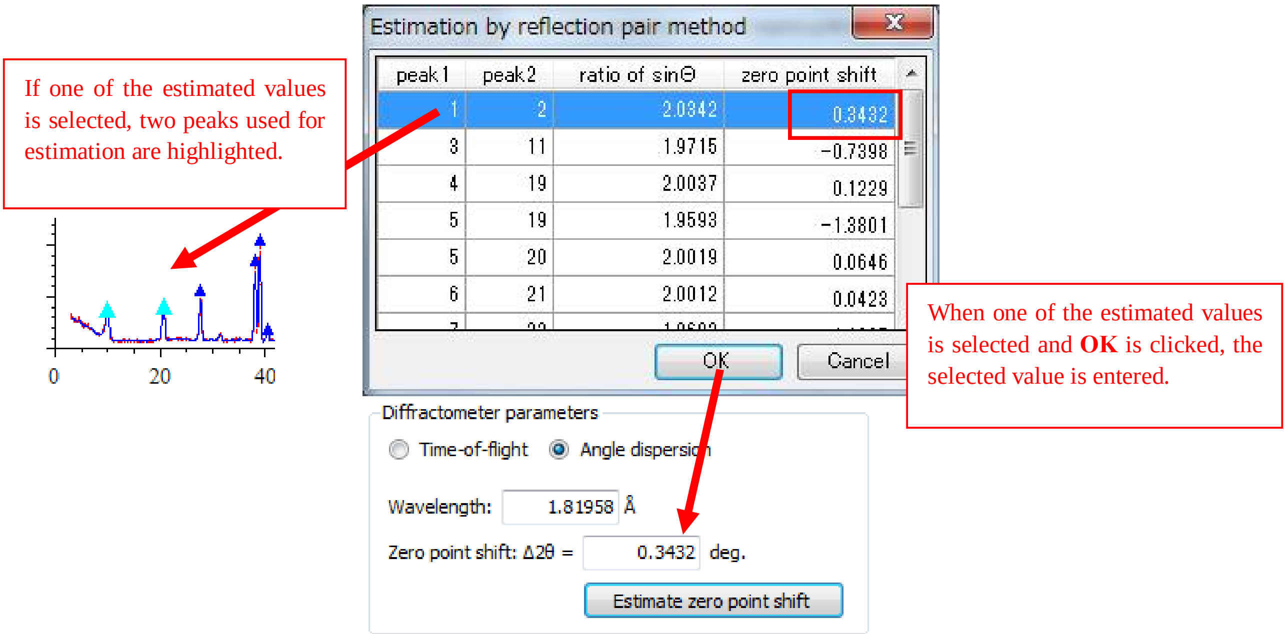


Fig. 4-4 Estimation of zero point shift

4.2. Advanced indexing parameters

The recommended values for the parameters in this frame are set automatically when a project is created. Although in general the values need not be changed, it should be noted that when they were determined the most difficult cases of powder indexing were considered. Hence, improvement, particularly in computation time, may be obtained by changing these parameters, as described in Section 10.2.

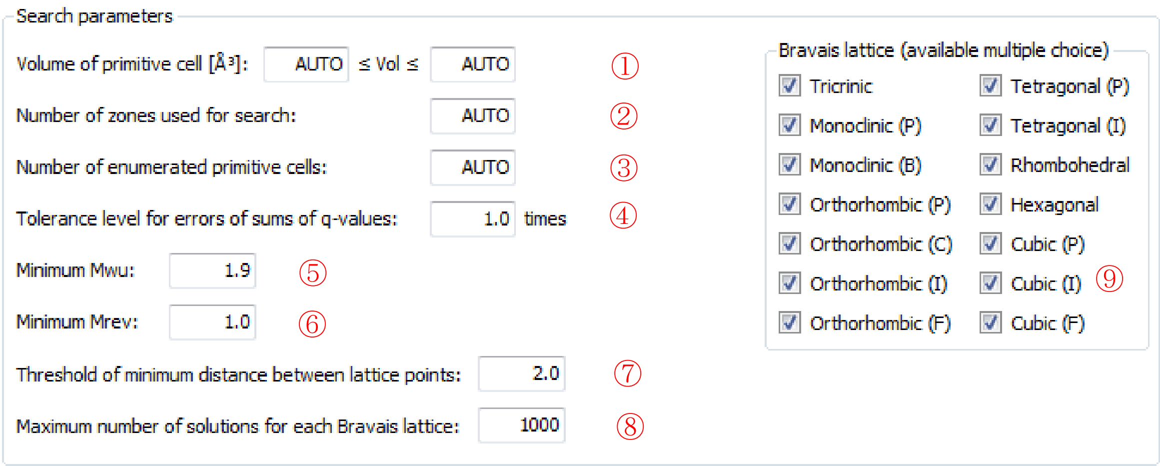


Fig. 4-5 Advanced indexing parameters

A description of the parameters and their recommended values are listed in Table 4-2.

Table 4-2 Advanced indexing parameters

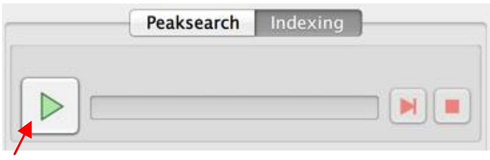
	Contents	Recommended value
①	Lower and upper limit of primitive cell volume	AUTO
②	Maximum value from four q values (= $1/d^2$) (q_1, q_2, q_3, q_4) acquired from selected topography that satisfies Ito equation	AUTO
③	Maximum number of powder indexing solutions to be enumerated (before Bravais lattice determination)	AUTO
④	Reference value to determine whether linear sum of q (= $1/d^2$) value is equal to zero, including Ito formula	1.0
⑤	Lower thresholds for the Wu FOM (M^{Wu}), the reversed FOM (M^{Rev}), and the distance between two closest points in the crystal lattice. If a solution has values below these thresholds, it is deleted, and cannot be retrieved after indexing is executed.	1.9
⑥		1.0
⑦		2.0
⑧	If a solution has a rank below this number when all the solutions with the same Bravais types are sorted in the order of the de Wolff FOM (M), it is deleted, and cannot be retrieved after indexing is executed.	1000
⑨	Untick the checkbox, if lattice parameter candidates of the Bravais type are NOT necessary.	☑(Yes)

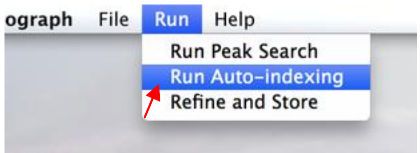
5. Indexing

After executing a peak search and setting diffractometer parameters, indexing can be started.

5.1. Indexing execution

To start indexing and obtain a list of lattice parameter candidates, click the ñRun indexingò button , or select **Menu > Run > Run auto-indexing** (the values of the input parameter are stored in the ***_pks.histogramIgor** and ***.inp.xml** files from the **auto_generated_files** folder):





While the indexing is being executed, the progress is outputted in the **Log Note** frame (Fig. 5-1). The Skip button  can be used only when searching a solution, and when it is clicked, the solution search is aborted and the program shifts to subsequent processing. On the other hand, the Cancel button  can be used at any time, and when it is clicked, the indexing is discontinued.

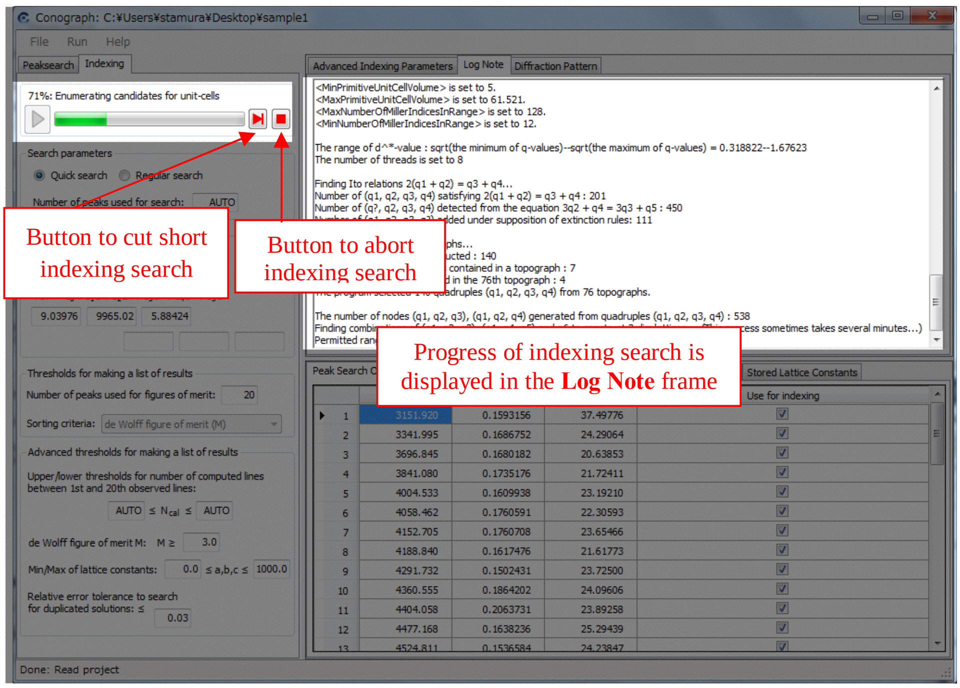


Fig. 5-1 Screenshot during indexing execution

5.2. When indexing is complete

When indexing is complete, the screen shown in Fig. 5-2 appears.

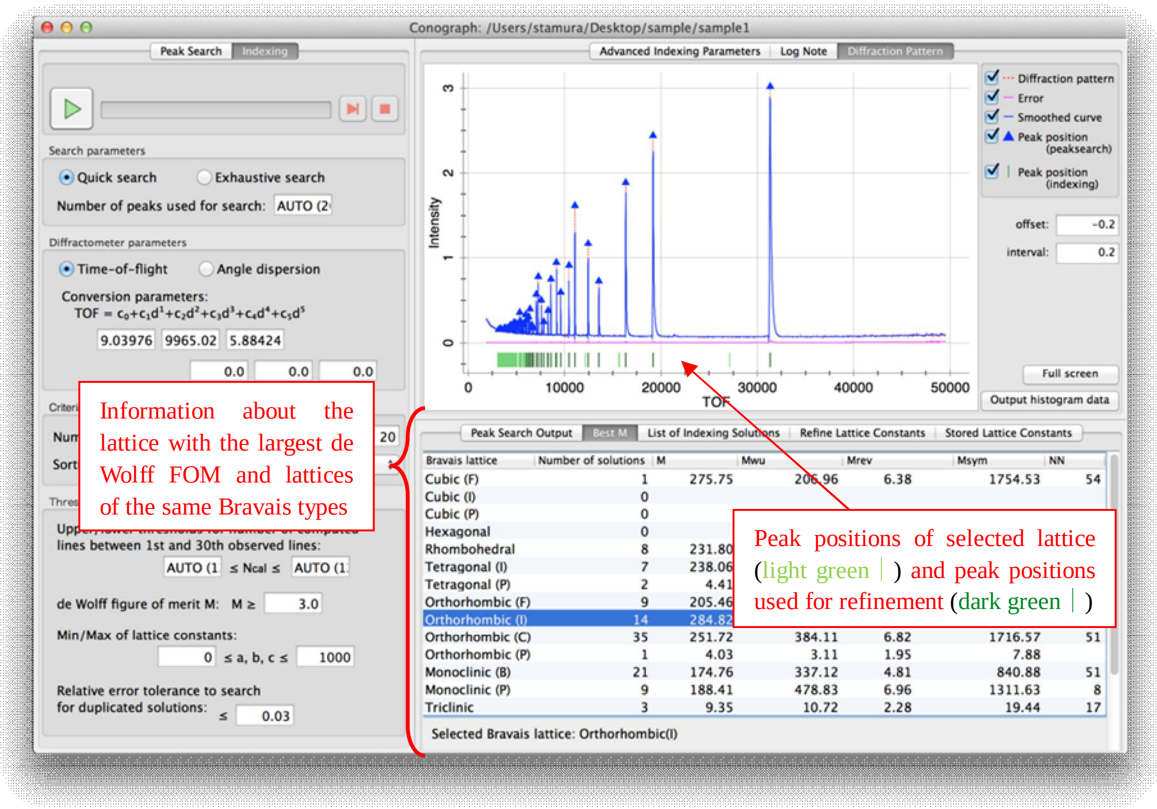


Fig. 5-2 Screenshot immediately after indexing execution

The lattice with the largest de Wolff FOM (Section 5.3) is automatically selected, and its information is displayed in the ñSelected Lattice Constantsò frame. In the **Diffraction Pattern** frame, the peak positions of the selected lattice are displayed with a light green tick mark (|). From these, the peak positions used for refinement (Chapter 6) are selected and displayed with a dark green tick mark (|).

5.3. Sorting /filtering lattice parameters

The lattice parameter candidates obtained by indexing can be sorted and filtered using parameters in the **Criteria for lattice parameters in candidate list** and **Advanced thresholds for lattice parameters in candidate list** areas of the **Indexing** frame.

The lattice parameters listed in the drop-down menu of the **Lattice Constants** frame are sorted and filtered using the parameters in the areas of Fig. 5-3. After indexing, sorting and filtering can be redone at any time, by changing the values of these parameters.

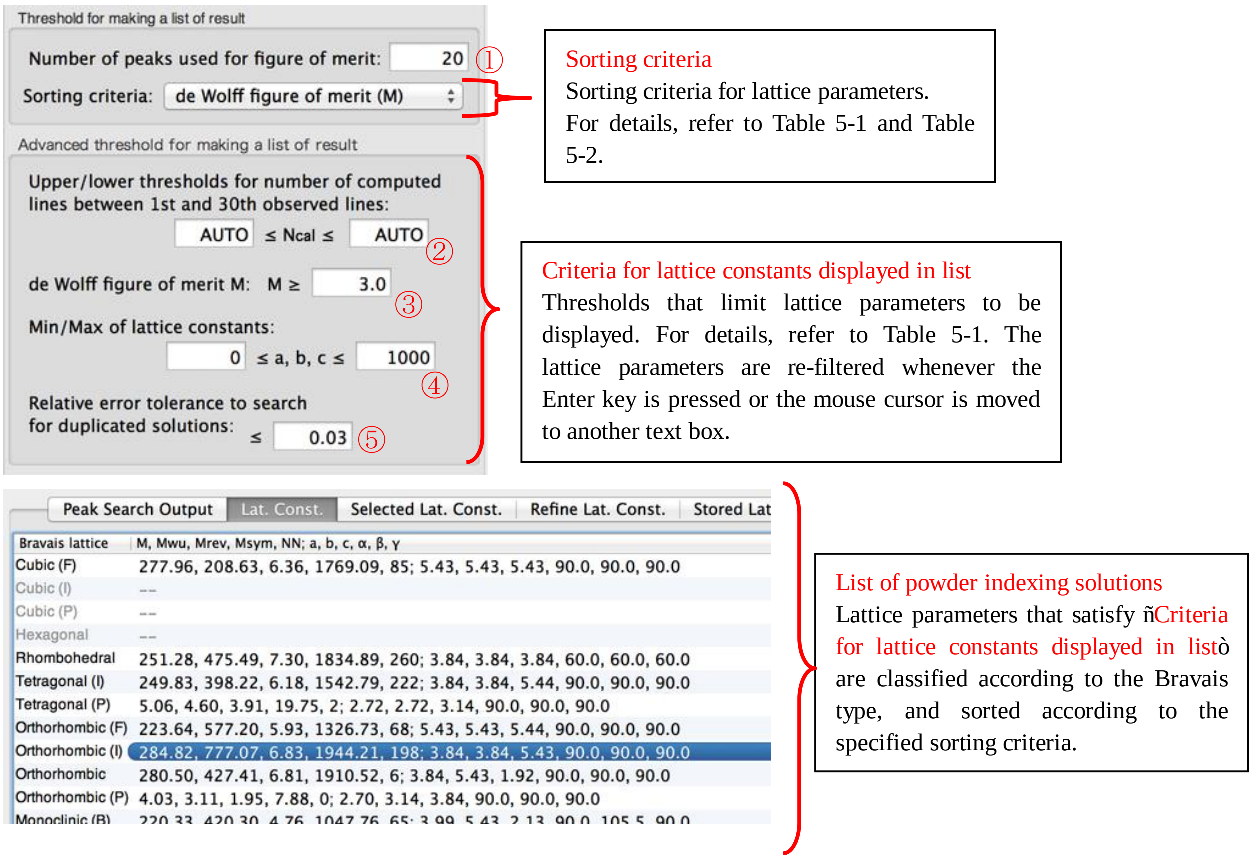


Fig. 5-3 Sorting criteria and thresholds for lattice parameters in candidate list

An explanation of the parameters and their recommended values are listed in Table 5-1. The recommended values are set up automatically in the text box when a project is created.

Table 5-1 Thresholds for lattice parameters displayed in candidate list

	Contents	Recommended value
①	Number of n peaks used for calculation of figures of merit (FOM). (The first n smallest q-values are used. This parameter can be larger than the number of peaks contained in the diffraction pattern, because it is automatically reduced.)	20
②	If the lattice parameters are specified, it is possible to calculate the number of peaks that exist in the range from the first to the n^{th} observed peaks. Lower and upper thresholds of the number.	AUTO
③	Only lattice candidates with a de Wolff FOM (M_n) greater than this value are displayed.	3
④	Lower and upper thresholds of lattice parameters a, b, c (Å).	
⑤	Relative resolution of d* (= 1/d) value. (Used for deciding whether two lattices are identical.)	0.03

Immediately after indexing is executed, lattice parameters in the list are sorted according to the de Wolff FOM (M_n). By using the **Sorting criteria** drop-down menu (Fig. 5-4), it is possible to change the sorting criteria for the lattice parameters (refer to Table 5-2).

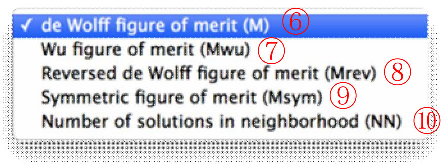


Fig. 5-4 Sorting criteria for lattice parameters

Among the aforementioned five FOM, the de Wolff FOM gives preference to the lattice parameters with high symmetry, and has the best efficiency. However, another FOM occasionally might be more effective than the de Wolff FOM, particularly if the powder diffraction pattern contains impurity peaks [5].

The first four FOM (⑥--⑨ in Table 5-2) are defined in such a way that the values become close to 1 if there is no correlation between the observed and computed lines. A lattice satisfying $M_n > 10$, $M^{Wu} > 10$, $M_n^{Rev} > 3$, or $M_n^{Sym} > 30$ is in general likely to be the correct solution. However, sometimes several distinct lattices may obtain large FOM values simultaneously. To select the most appropriate lattice parameters, all the plausible solutions should be checked using the methods described in Sections 5.4 and 5.5.

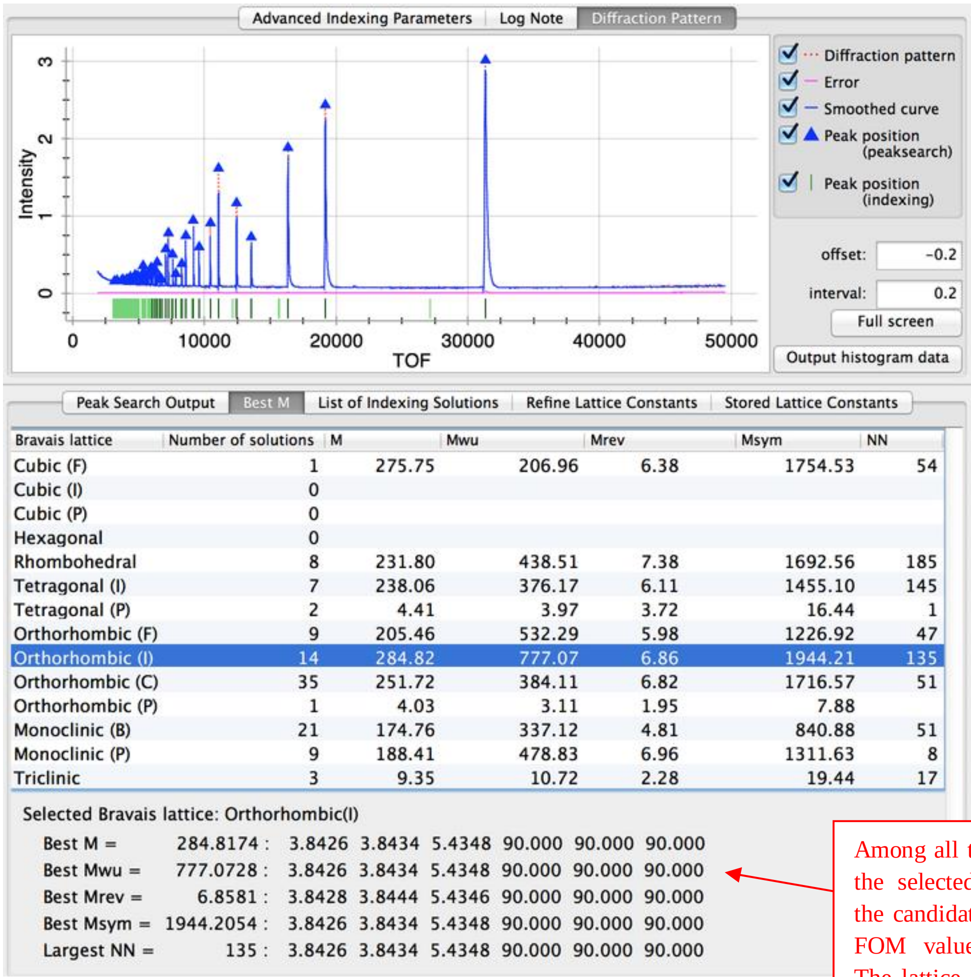
Table 5-2 Sorting criteria for lattice constants displayed in list

⑥	Sort in descending order by the de Wolff FOM (M) [6] (computed by using the method described in [5] to increase the numerical stability). The de Wolff FOM possesses these properties: a) Insensitive to existence of unobserved computed lines (according to extinction rule) b) Sensitive to existence of un-indexed observed lines (such as impurity peaks) c) When almost identical lattices belong to different Bravais types, the lattice with higher symmetry normally obtains a higher value.
⑦	Sort in descending order by Wu FOM (M^{Wu}) [7]. In terms of a) and b), it is similar to the de Wolff FOM; in terms of c), it is opposite, that is, a lattice with a lower symmetry is more likely to obtain a high value.
⑧	Sort in descending order by Reversed FOM (M^{Rev}) [5]. M^{Rev} is computed by exchanging the roles of observed peak positions and calculated peak positions in the definition of the de Wolff FOM. Because of this, it has properties that are opposite to those of the de Wolff FOM: aô) Sensitive to existence of unobserved computed lines bô) Insensitive to existence of un-indexed observed lines cô) Tends to select a lattice with lower symmetry As in the case of the de Wolff FOM, if there is no correlation between observed lines and computed lines, the value becomes close to one.
⑨	Sort in descending order by Symmetric FOM (M^{Sym} = M M^{Rev}) [5]. According to its definition, it has properties between ⑥M and ⑧M^{Rev}. As in a number of statistical quantities, such as chi-squares or R factors, the value remains the same after observed lines and computed lines are exchanged
⑩	Sort in descending order by NN (=number of lattices judged to be almost identical among all the solutions, by using the relative resolution in ⑤).

5.4. Find plausible indexing solutions

Several of the FOM introduced in Section 5.3 can extract a small number of candidates with high compatibility with inputted peak positions from multiple powder indexing solutions. However, none of the FOM is sufficiently effective when two lattices that belong to different Bravais types are compared. In order not to miss plausible solutions, in addition to their values of FOM, their Bravais types should be checked.

By using **Best M Frame**（Fig. 5-5）, it is possible to compare the best FOM values of the solutions in each Bravais type. By clicking the name of a Bravais types, the solutions with the largest FOM are displayed.



Among all the lattices with the selected Bravais type, the candidate with the best FOM value is displayed. The lattice can be selected by clicking on it.

Fig. 5-5 Best M frame

In order not to spend much time searching for plausible solutions, you should check the information displayed in **Best M frame** in terms of the following two points:

(i) Which Bravais types include a solution with a fairly large de Wolff FOM (M_n) lattice (for

example, $M_n > 10$)?

(ii) Among all the lattices of such a Bravais type, does the same lattice obtain the maximum value in almost all FOM, including the de Wolff FOM? This is because different FOM have complementary properties (refer to Table 5-2), and therefore, a lattice that has obtained the maximum values for M_n, M_n^{Rev}, and M_n^{Sym} has a high possibility of being the true solution.

By clicking on a set of lattice parameters in **Best M Frame** (Fig. 5-5), the tick marks in the **Diffraction Pattern frame** are automatically updated, and information about the parameters is displayed in the **Selected Lattice Constants** frame (Fig. 5-6, Table 5-3).

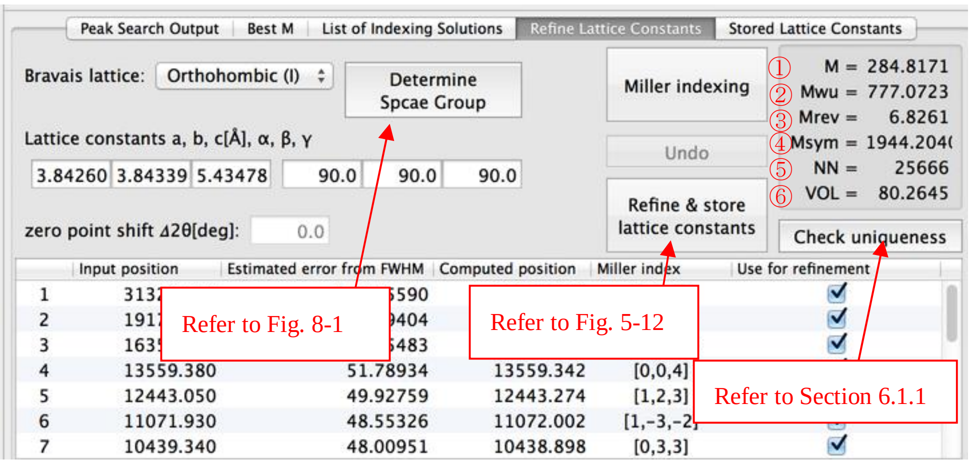


Fig. 5-6 Selected Lattice Constants frame

Table 5-3 Information displayed in Selected Lattice Constants frame

①	Value of the de Wolff FOM (M) of the selected lattice
②	Value of Wu FOM (M^{Wu}) of the selected lattice
③	Value of Reversed FOM (M^{Rev}) of the selected lattice
④	Value of Symmetric FOM (M^{Sym}) of the selected lattice
⑤	Value of NN of the selected lattice, *i.e.*, the number of lattices that are found during indexing execution and judged to be identical with the selected lattice.
⑥	Unit-cell volume (Å^3) of the selected lattice

All the lattice parameters saved during the execution of powder indexing are displayed in **Lattice Constant Frame** (Fig. 5-7). It is possible to check peak positions of all the solutions in **Lattice Constant Frame** by scrolling them, using the up and down arrow keys or the mouse wheel. By clicking the name of a Bravais type in **Lattice Constant Frame**, the solution with the largest FOM (specified in **Indexing Frame**) is selected:

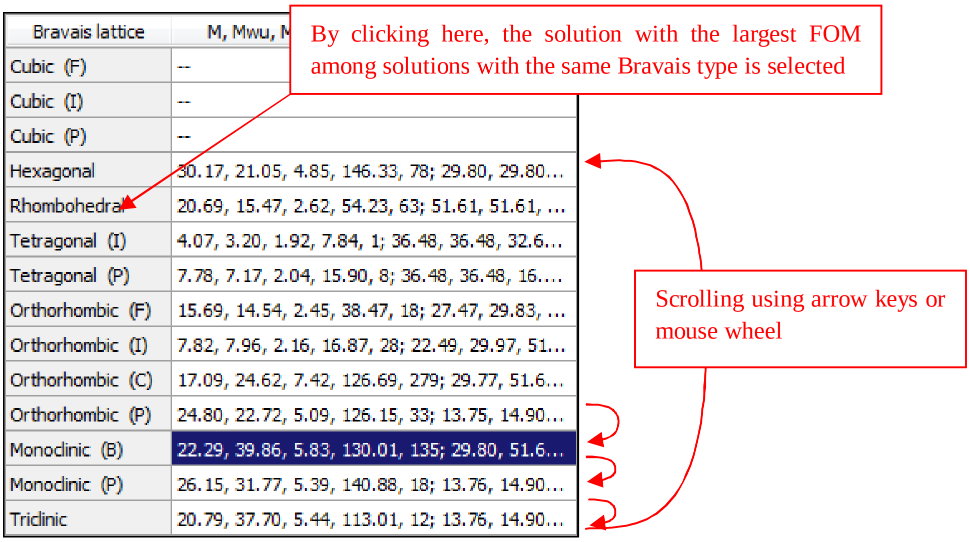


Fig. 5-7 List of lattice parameter candidates obtained by indexing

It should be noted that the values of the FOM are occasionally improved greatly by refinement (Fig. 5-8). The operations necessary for refinement are explained in Section 6.1.1.

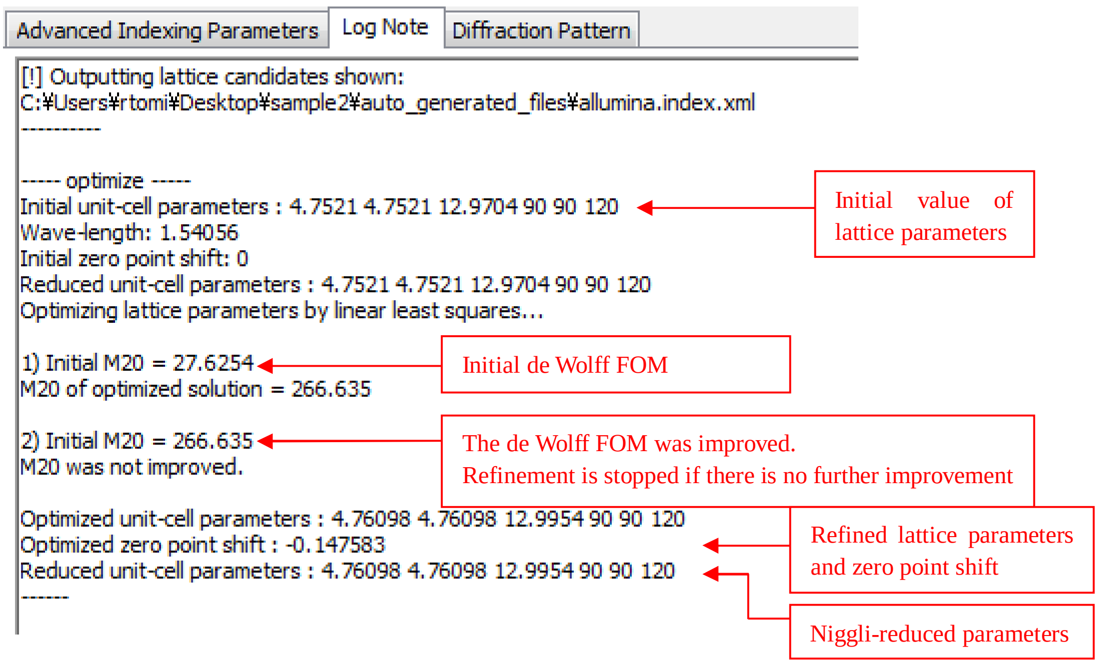


Fig. 5-8 Message outputted in Log Note frame during refinement execution

While the refinement is being executed, a warning concerning dominant zones may appear in the **Log Note** frame (Fig. **5-9**). When this warning appears, it may be considered that the FOM did not work efficiently. Therefore, it is advisable to increase the <Number of peaks used for computation of

FOM> in the **Criteria for lattice constants in the list** area (Fig. 5-3), according to the warning. Next verify that there is no warning when refinement is executed again.

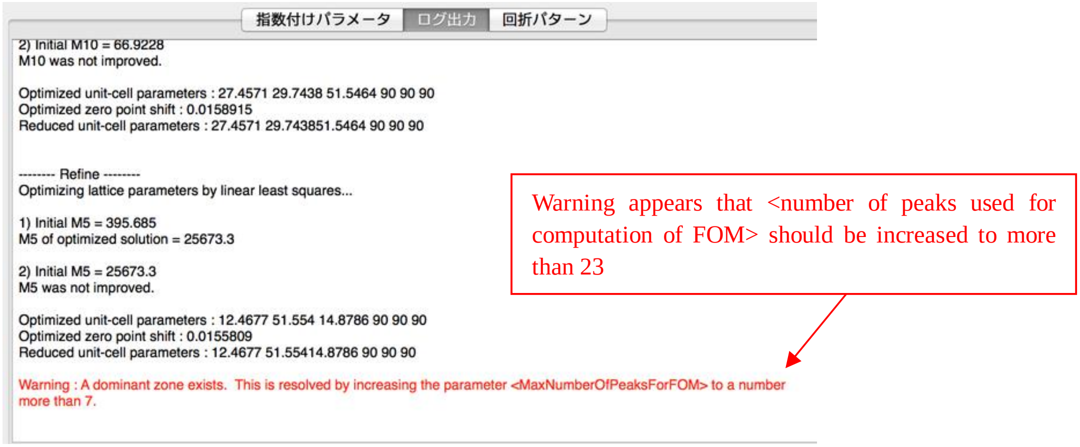


Fig. 5-9 Log message reporting that a dominant zone is found

5.5. Decide the correct lattice parameters

Before drawing a conclusion as to which solution for the lattice constants is correct, the computed lines (|) and the observed lines (z) should be compared. In addition, the lattice parameters may not be determined uniquely from the peak positions (Fig. 5-10). This phenomenon occurs infrequently in low-symmetry cases and consistently in high-symmetry cases, and is known as *geometrical ambiguity* [2]. Therefore, it should be checked in respective cases whether or not the uniqueness of solutions holds by using Conographôs **Check Uniqueness** button (Fig. 5-12).

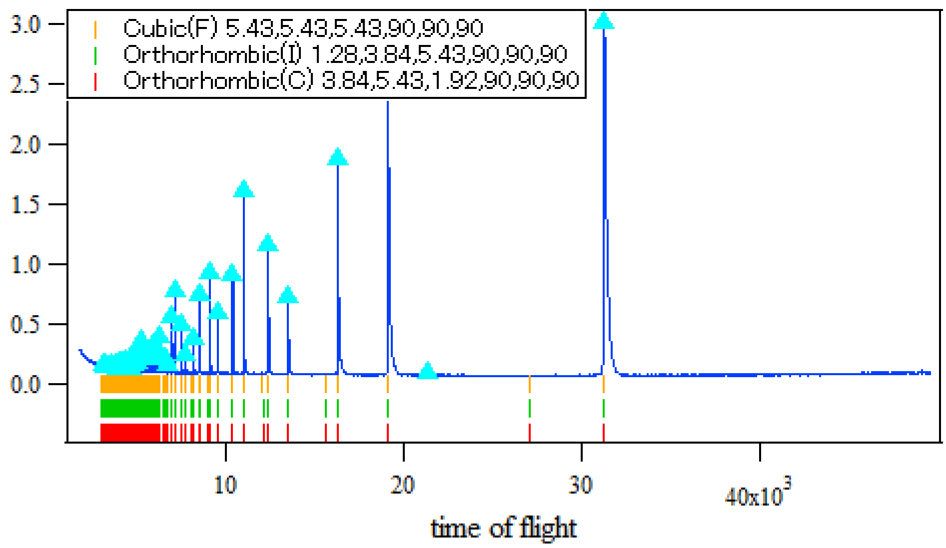


Fig. 5-10 Example of distinct lattice parameters with identical peak positions

The peak positions of all the lattices that have been refined can be displayed as tick marks on the **Diffraction Pattern** frame. This allows the peak positions (|) of several lattice parameters to be compared simultaneously. In order to hide tick marks of some of the lattices, untick the corresponding check boxes labeled **Plot** (or the corresponding lattice can be deleted) in the **Stored Lattice Parameters** frame.

The methods for changing the display of tick marks are shown in Fig. 5-11 and Table 5-4.

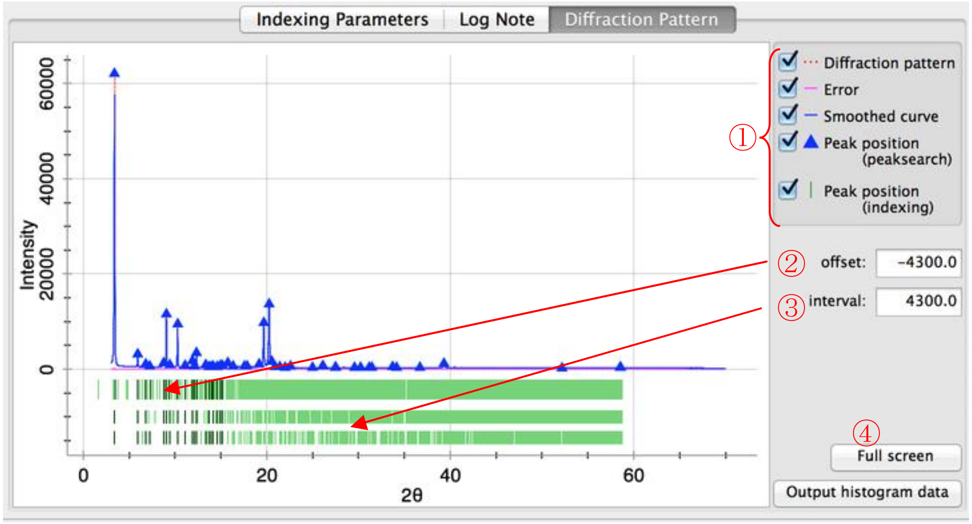


Fig. 5-11 Diffraction Pattern frame

Table 5-4 Diffraction Pattern frame

①	Displays/hides switch
②	Height (y-coordinate) of the position of tick marks displayed at the top. Press Enter key to reflect the change. This height can be increased or decreased by locating the cursor in the text box and rotating the mouse wheel.
③	Space between tick marks and tick marks immediately below
④	Enlarges the **Diffraction Pattern** frame to full screen.

If the peak positions of a solution accord well with the observed lines in the diffraction patterns, select the solution and click the **Check Uniqueness** button. Then, all the lattices with almost the same peak positions as the currently selected lattice are generated [3].

If such lattices exist, a window appears as shown in Fig. 5-12. The available operations in the window are the same as in the **Diffraction Pattern** frame. By clicking the ñOutput histogram dataò button, a histogram file that contains the peak positions of all the lattice parameters displayed is outputted.

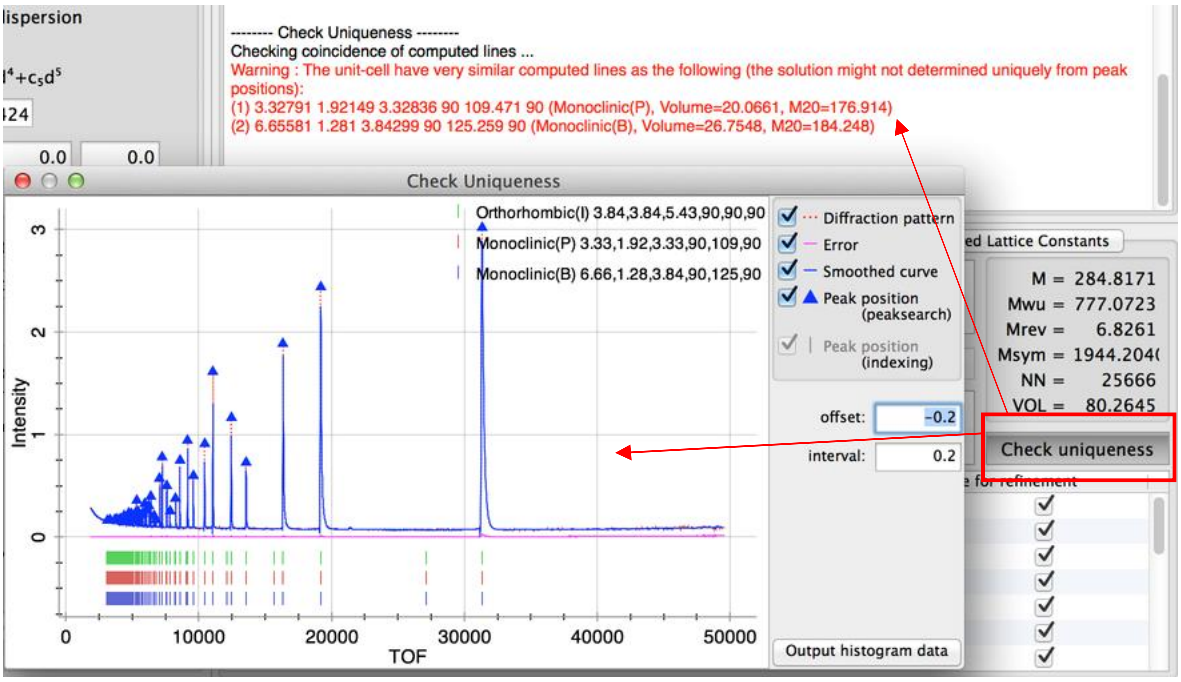


Fig. 5-12 Check uniqueness of solutions

6. Refining lattice parameters and zero point shift

The method for refining lattice parameter candidates obtained by indexing (and zero point shift for angle dispersion methods) is explained in the following sections. The refinement is conducted using linear/non-linear least squares methods.

6.1. Method for refinement execution

6.1.1. Refinement of lattice parameters selected from the list

To refine the lattice parameters and zero point shift, select the lattice parameters and then click the **Refine & store lattice constants** button in the **Refine Lattice Constants** frame (or by selecting **Menu > Run > Refine & store lattice constants**):

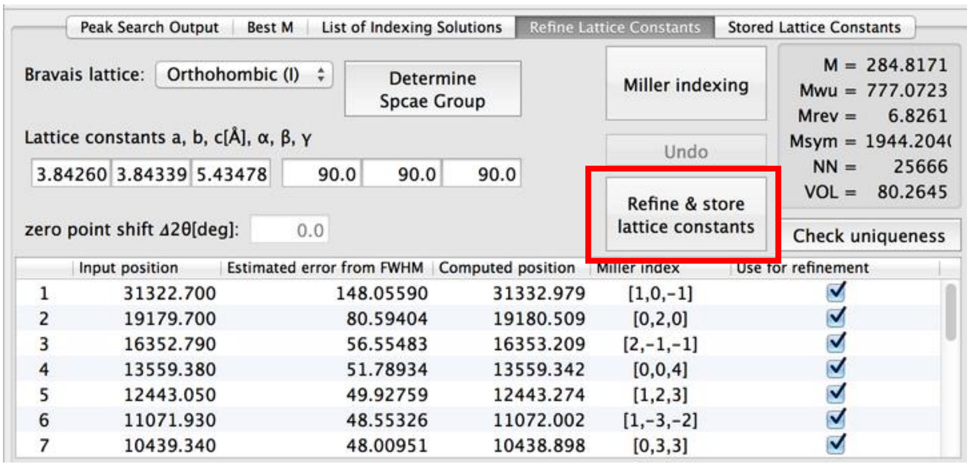


Fig. 6-1 shows a screenshot when the refinement is being executed. The refined lattice parameters are saved and displayed in the **Stored Lattice Constants** frame.

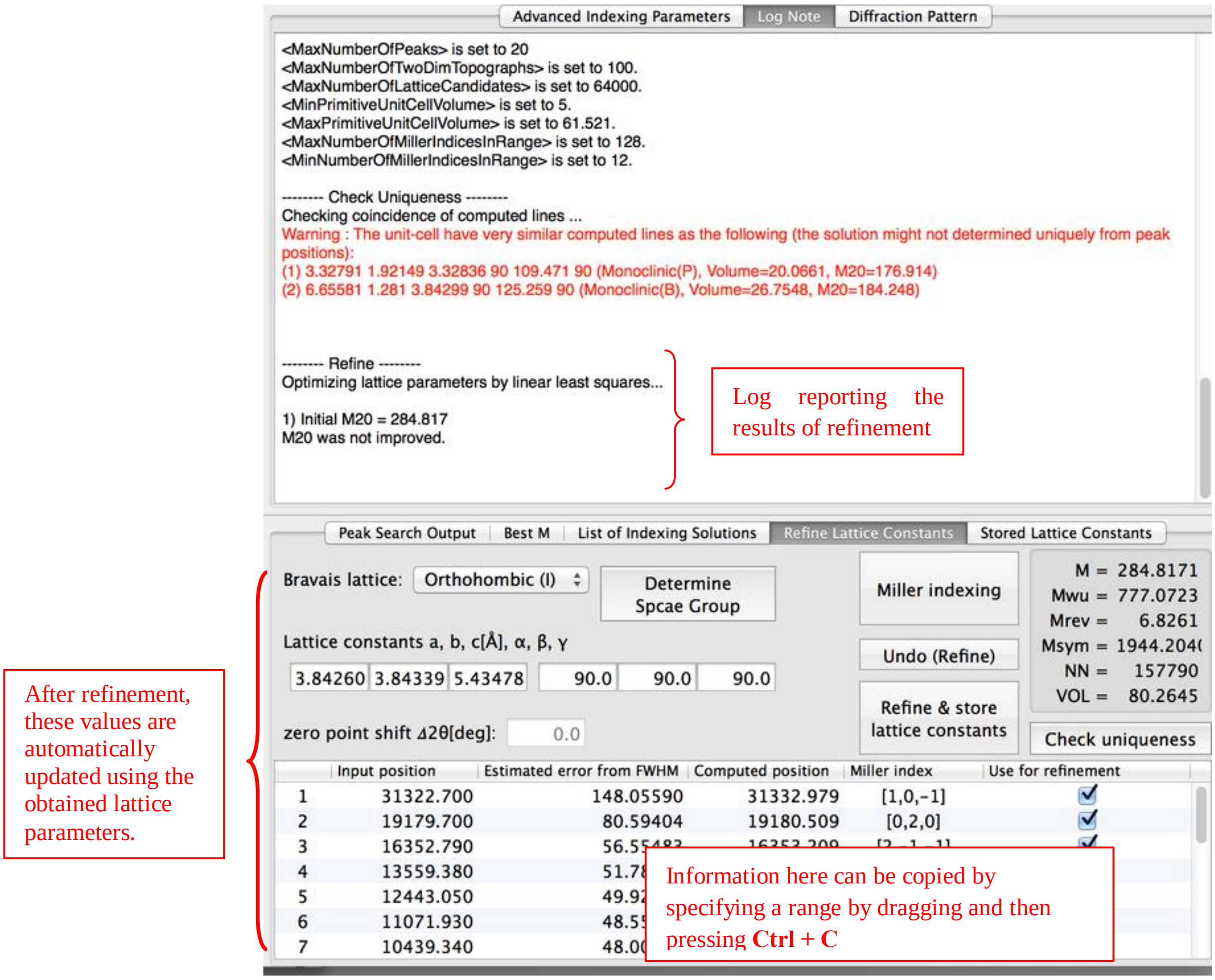
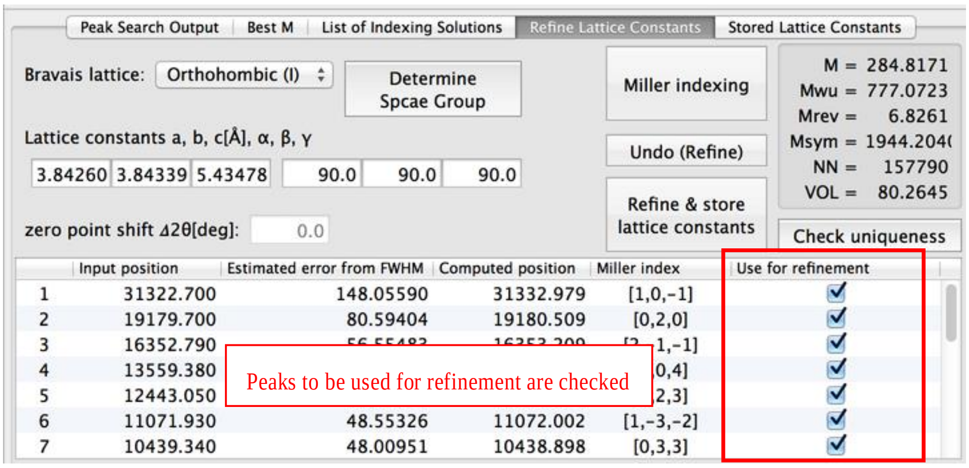


Fig. 6-1 Screenshot during refinement execution

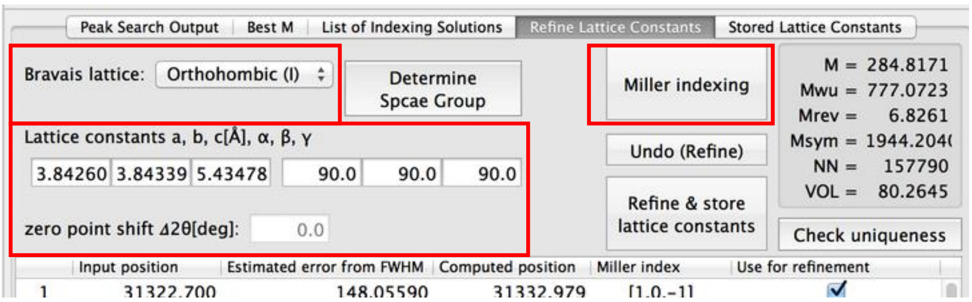
The peak positions to be used for refinement can be selected manually from the **Use for refinement** column in the **Refine lattice constants** frame. The color of a tick mark changes from dark green (|) to light green (|), according to a change in the corresponding flag.



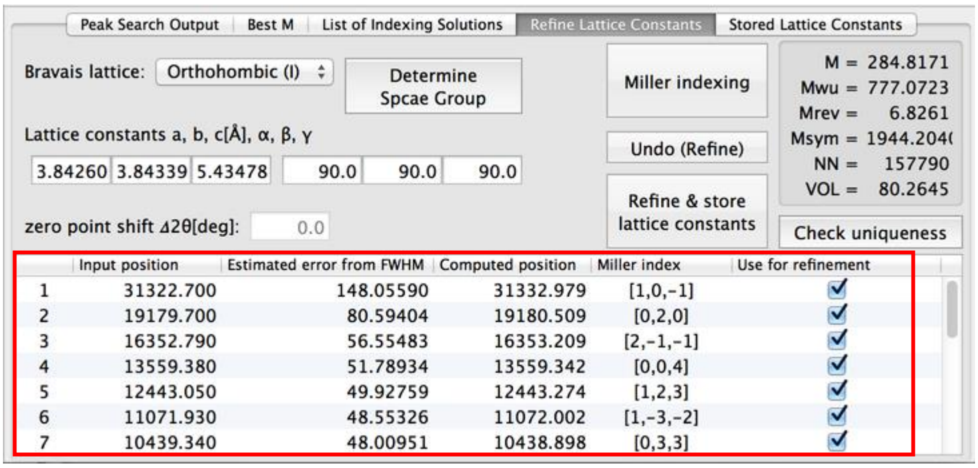
6.1.2. Refining lattice constants entered by user

This section explains the method for refining lattice parameters specified manually by the user. In this case, although indexing execution is not required for refinement, a peak search is required for obtaining peak positions.

The diffractometer parameter **Wavelength of diffractometer** (or **Conversion Parameters**) can be inputted from the **Indexing** frame. When the angle dispersion is selected, it is also possible to enter an initial value of the zero point shift from the **Refine lattice constants** frame (normally, it is not necessary to set the initial value to a value other than 0):



If the **Miller indexing** button is clicked, the Miller indexing of peaks is performed using the Bravais lattice and lattice parameters entered. Subsequently, the Miller indices assigned to peaks are displayed:



The refinement of the lattice parameters is performed using the assigned Miller indices. If required, it is possible to manually specify which peak positions are to be used for refinement, by using the flags in the rightmost column (refer to Table 6-1 for the meaning of the other columns). When the **Refine & store lattice constants** button is clicked, lattice parameters are refined, and appended in the **Stored Lattice Constants** frame.

Table 6-1 Information about peaks in Refine lattice constants frame

Column	Contents
1	Peak positions of the considered diffraction pattern
2	These values (calculated from the full widths at half maximum of peaks) are used as weights for least squares method
3	Peak positions of the selected lattice constants computed by using the Miller indices in column 4 and diffractometer parameters
4	Miller indices used for refining lattice parameters
5	Checked, if the peak position is used for refining lattice parameters

6.2. **Undo** button

By clicking the **Undo** button, it is possible to restore the lattice parameters and the zero point shift to the values that existed before you keyed in the numbers in the text boxes or executed refinement (Fig. 6-2). This **Undo** cannot be applied successively, and therefore, only the last values of the parameters can be retrieved.

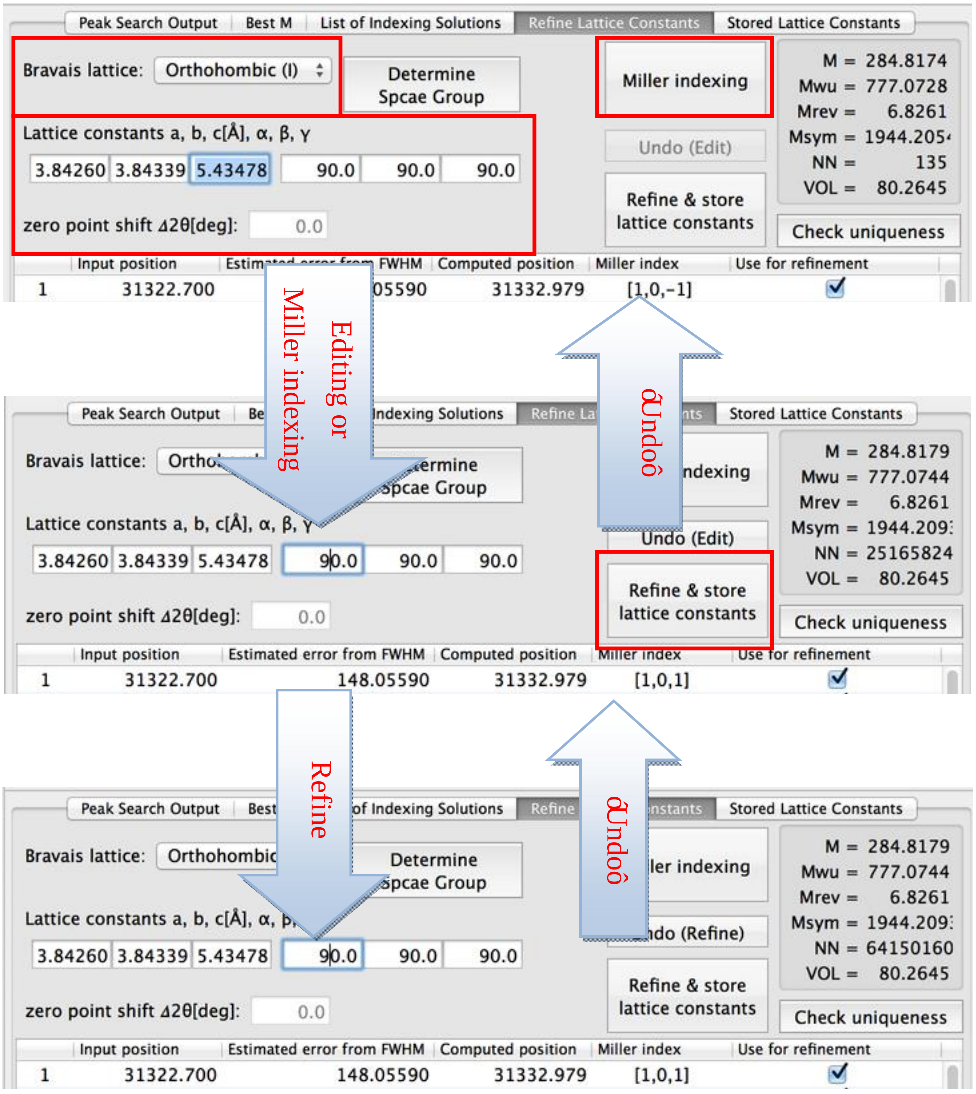


Fig. 6-2 Undo button

7. Result output

There are three types of output files, ***.index.xml** (***.index2.xml**), ***.histogramIgor,** and a backup file (all are text files, except for the backup file). The respective output files are explained in the following sections.

7.1. *.index.xml

The **auto_generated_files/*.index.xml** file is outputted in the project folder, if either of the following events occurs:

- Indexing execution is completed
- The application is closed or another project is started
- **File > Output all lattices** (Fig.7-1) is selected.

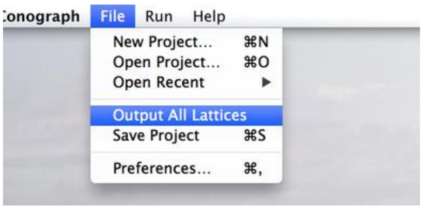


Fig.7-1 Output all lattices

From the lattice parameter candidates obtained by indexing, the lattice constant information displayed on the GUI is indicated in the ***.index.xml** file (for the format, refer to Fig. 11-5 and 10-7). If the name of the diffraction data file is ***.histogramIgor**, the name of the output file becomes ***.index.xml.** The same file is always overwritten at the time of the above events.

7.2. Igor text file and *.index2.xml file

When the **Output histogram data** button (Fig.7-2) is clicked, the ***.histogramIgor** file is outputted in the project folder. In this file, in addition to the contents of the input diffraction data file, the Miller indices and the peak positions of the lattice parameters that show tick marks in the **Diffraction Pattern** frame are saved.

Output ***.histogramIgor** file containing Miller indices and their corresponding peak positions (tick marks)

Fig.7-2 Output of Igor file

At the same time, information about the lattice parameters outputted in the ***.histogramIgor** file is outputted as the ***.index2.xml** file.

7.3. Backup file

When **File > Save project** (Fig. 7-3) is selected, a backup file is created in the folder as the **auto_generated_files/backup.dat** file, which stores all the lattice parameter candidates that were obtained by indexing or exist in the **Stored Lattice Constants** frame.

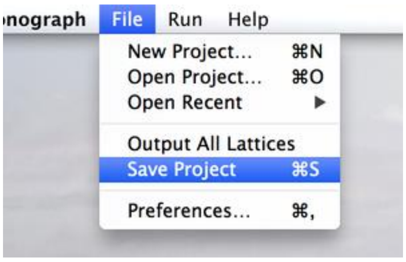


Fig. 7-3 Saving a project

This file is also outputted when a project containing a data set of lattice parameters is closed (this occurs when the application is closed or another project is opened).

By using the backup file, the condition at the time of saving **backup.dat** can be reproduced when Conograph is started in the next session. When the project is opened in the next session, the user is asked whether s/he wishes to open the backup file, if it exists in the project folder. The existing backup file is overwritten whenever either of the above events occurs in the opened project.

8. Space group determination

In the stages described thus far, only the systematic absences caused by the Bravais lattice type were considered during computation of the figures of merit. However, additional extinction derived from the space group may have happened. If the **Determine Space Group** button in the **Refine Lattice Constants** frame is clicked, the value of the de Wolff figure of merit M is recomputed by using the reflection conditions of each space group with the Bravais lattice type selected in the frame, and a window as in Fig. 8-1 appears. The M values of all the space groups are listed up in the window, and it is possible to check which space group fits well to the observed peaks.

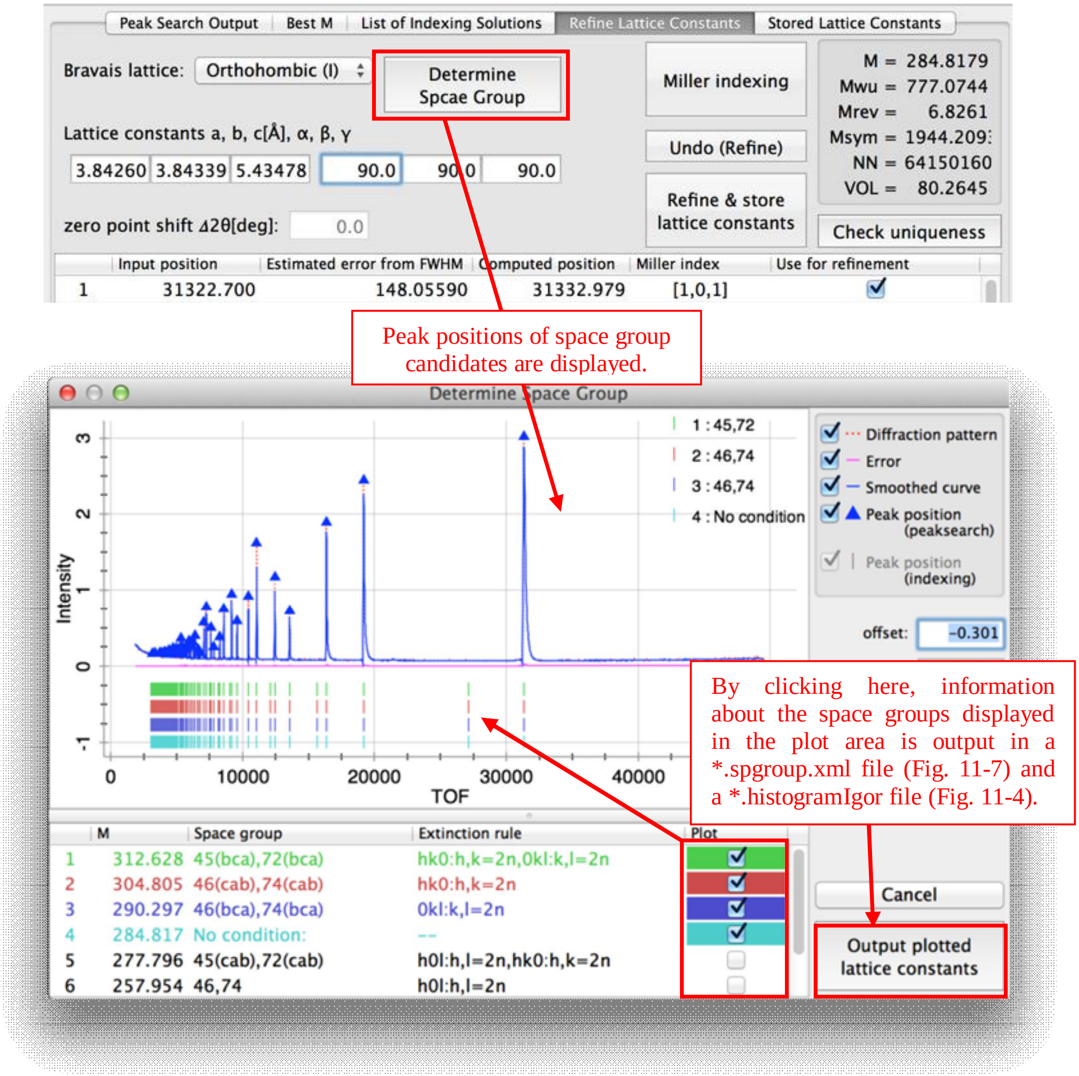
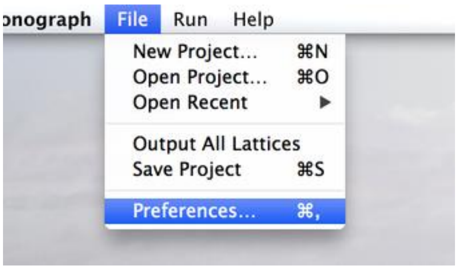


Fig. 8-1 Determination of space group candidates

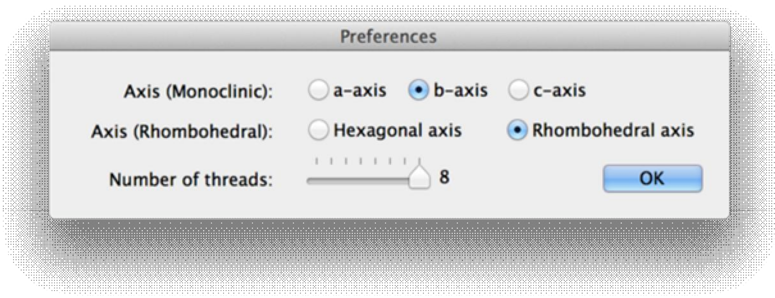
9. Other GUI operations

9.1. Configuration parameters

Select the **Menu > File > Preferences** as follows:



Then, the following **Environment variables settings** dialog box is displayed.



The <Number of threads> is used when running parallel computing. The number to which this parameter can be set depends on the computer. The initial value is set to (the number of threads the computer has) - 1. The higher the value, the greater is the speed; however, the computational cost also becomes high. It is advisable to set a small value if you want to run another application simultaneously.

The used configuration parameters are stored in the **auto_generated_files/*.inp.xml** file. The values of the configuration parameters when the application is closed are stored in the software setup file and are reset when the next session starts.

9.2. Help menu

From the **Help** menu, you can select **Manuals**:

When **Manual** is selected, the user manual (*i.e.*, this manual) appears.

10. Parameters that can be changed to obtain better results

10.1. Peak search

In peak search, it is recommended that diffraction peaks are collected as uniformly as possible on the basis of peak height. Filtering diffraction peaks manually (including removal of overlapped peaks) is unnecessary and not desirable, unless there is valid prior information.

In order to obtain such a peak search result, only the following parameters need to be adjusted:

(1) <Threshold for peak height>

(2) <Number of data points used for smoothing histogram>.

In addition, in cases of characteristic X-ray data that contain $\alpha 2$ peaks, the $\alpha 2$ peaks must be removed prior to powder indexing (Fig. 3-1).

The following are notes related to the adjustment of the parameters (1) and (2).

(1) <Threshold for peak height>

This parameter is used as a lower threshold for magnitudes of intensities to be detected in a peak search. If **c×(error value of intensity)** is used, as in the default setting, a peak at peak-position x is detected, if and only if it has a peak height greater than (the threshold) × Err[y], where Err[y] is the value of the error in intensity at x. The peak height used here is obtained by subtracting the estimated background value from y. Our recommended threshold value is within the range of 3ð 10.

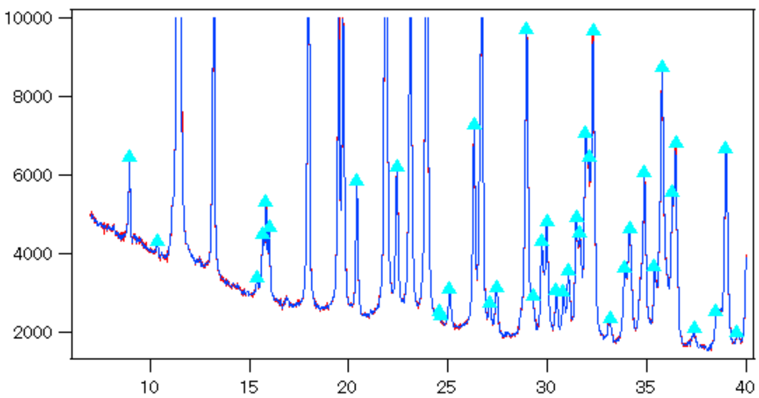


Fig. 10-1 Example of peak search results in radiation beam data

(2) <Number of data points used for differential calculation>

This parameter can be used to avoid background noise being picked up as peaks. If it has a small value, the smoothing curve is fit more finely to local irregularity, because the number of data points for computing each y-value of the smoothing curve is set to this value. Fig. 10-2 shows an example.

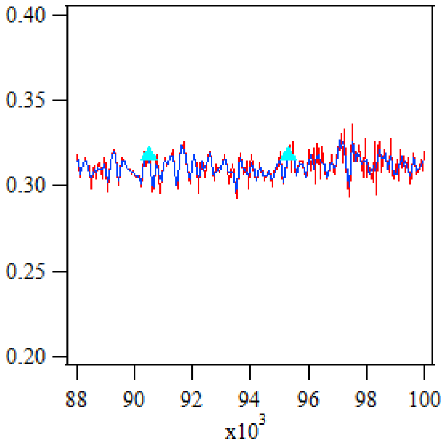


Fig. 10-2 <Number of data points> = 5

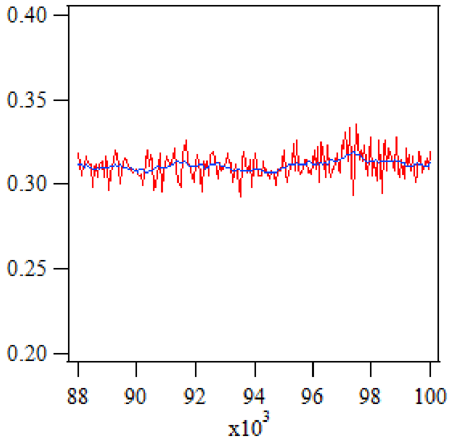


Fig. 10-3 <Number of data points> = 25

10.2. Powder indexing

It has been confirmed that a search using the recommended parameter values provides correct solutions in an extremely wide range of cases, in particular, in memory-efficient search [4]. Nevertheless, if good results are not obtained, they may be improved by changing some of the parameters. In the following, the parameters to be changed in order to conduct a more exhaustive search (Section 10.2.1), enhance computing speed (Section 10.2.2), and improve the efficacy of the figures of merit (Section 10.2.3) are explained.

10.2.1. Conduct a more exhaustive search

(1) <Searching method> in **Indexing** frame: **Quick search** ⇒ **Exhaustive search.**

(2) <Number of peaks used in the search> (**Indexing** frame): **AUTO** ⇒ a number greater than 48

When **AUTO** is entered, 48 peaks are used for powder indexing, unless the diffraction pattern contains only a smaller number of peaks. However, even this number of peaks may be insufficient if a dominant zone exists. In such cases, increasing the number is effective.

(3) <Tolerance level for errors of sums of q values> (**Advanced Indexing parameter** frame): 1 ⇒ 1.5

In cases of characteristic X-rays or reactor sources, better results may be yielded if a large value is used.

10.2.2. Enhance computing speed

(1) Increase <Number of threads> (**File > Preferences**)

The simplest method is to increase the number of threads used.

(2) <Search parameters> (**Indexing parameters** frame): **Exhaustive search** ⇒ **Quick search**.

(3) <Bravais lattice> (**Advanced Indexing Parameters** frame): untick

If you have prior information about the Bravais type, the information can be used to reduce the time required in the stage after Bravais lattice determination.

(4) Increase values of <Volume of primitive cell> or <Thresholds of minimum distance between lattice points> (**Advanced Indexing Parameter** frame)

If you have prior information about these parameters, the information can be used to reduce the time required for powder auto-indexing.

10.2.3. Improve the efficacy of figures of merit

(1) <Zero point shift> (**Indexing** frame): 0 deg. ⇒ more accurately estimated value

For diffraction patterns with a large zero point shift (æ2θ > approximately 0.1°), the FOM values sometimes become small. The results may be improved by conducting powder indexing using the estimated value of the zero point shift. The zero point shift can be estimated by using one of the following methods.

(a) The reflection pair method [1],

(b) After conducting powder indexing once, refine the zero point shift and lattice parameters with relatively larger M_n^{Rev} and M_n^{Sym} (for instance, $M_n^{Rev} > 3$ or $M_n^{Sym} > 10$ approximately), and re-execute indexing, using the obtained zero point shift.

In both methods, it is necessary to test several candidate values.

(2) <Number of peaks used for computation of FOM> (**Indexing** frame): 20 ⇒ a number greater than 20

The value 20 frequently used for this parameter might be insufficient if a problem called dominant zone occurs. If a dominant zone is found when refining the lattice constants and zero point shift, a warning message and the number of peaks required appear in the **Log Note** frame. In that case, set this parameter to a value greater than the number displayed.

(3) Improve results of peak search (or change the <Use for Indexing> flags in **Peak search output** frame)

Impurity peaks greatly affect the sorting results. Because of this, it is desirable to reduce the number of impurity peaks as far as possible, at least in the range of the first to n-th peaks, when the parameter <Number of peaks used for computation of FOM> is set to n.

11. Input/output text file formats

The formats for the input/output text files, cntl.inp.xml, *.inp, *.histogramIgor, and *.index files, are shown in this section.

```
<ZCodeParameters>
   <ConographInputFile>
      <!-- Control parameters for calculation.-->
      <ControlParamFile> HRP000675.BS.bin04f.inp.xml </ControlParamFile>
      <!-- Peak-position data.-->
      <PeakDataFile> HRP000675.BS.bin04f_pks.histogramIgor </PeakDataFile>
      <!-- Output file -->
      <OutputFile> hrp000675.bs.bin04f.index </OutputFile>
   </ConographInputFile>

   <PeakSearchInputFile>
      <ControlParamFile> HRP000675.BS.bin04f.inp.xml </ControlParamFile>
      <HistogramDataFile>
         <FileName> HRP000675.BS.bin04f.histogramIgor </FileName>
         <!-- "XY": general, "IGOR":IGOR; "Rietan":Rietan.-->
         <Format> IGOR </Format>
         <!-- When "IsErrorContained" equals 1, input errors in the 3rd column of the histogram.-->
         <IsErrorContained> 1 </IsErrorContained>
      </HistogramDataFile>
      <Outfile> HRP000675.BS.bin04f_pks.histogramIgor </Outfile>
   </PeakSearchInputFile>
</ZCodeParameters>
```

Fig. 11-1 Example of cntl.inp.xml

```xml
<?xml version="1.0" encoding="UTF-8" ?>

<ZCodeParameters>
  <ConographParameters>
    <!-- Parameters for the histogram.-->
    <!-- 0:tof, 1:angle dispersion-->
    <IsAngleDispersion> 0 </IsAngleDispersion>

    <!-- Conversion parameters for tof : a polynomial of any degree -->
    <ConversionParameters> 0 1 0        </ConversionParameters>

    <!-- Peak shift parameters for angle dispersion : Z(deg.), Ds(deg.), Ts(deg.).
         2*d*sin(theta0) = Wlength, 2*theta = 2*theta0 + Z + Ds*cos(theta0) + Ts*sin(2*theta0). -->
    <PeakShiftParameters> 0 </PeakShiftParameters>

    <!-- Wave length(angstrom) for angle dispersion. -->
    <WaveLength> 1.54056 </WaveLength>

    <!-- Parameters for search.-->
    <SearchLevel>
    <!-- 0:quick search (suitable for lattices with higher symmetries.),
         1:exhaustive search (suitable for lattices with lower symmetries.).-->                    0
    </SearchLevel>

    <!-- Number of reflections for calculation.-->
    <MaxNumberOfPeaks> AUTO </MaxNumberOfPeaks>

    <!-- The critical value c to judge if linear sums of Q equal zero. ( abs(¥sigma_i Q_i) <= c * Err<¥sigma_i Q_i> ) -->
    <CriticalValueForLinearSum>                1 </CriticalValueForLinearSum>

    <!-- Minimum of the volume of primitive unit-cell (>=0) -->
    <MinPrimitiveUnitCellVolume>            AUTO </MinPrimitiveUnitCellVolume>

    <!-- Maximum of the volume of primitive unit-cell (>0) -->
    <MaxPrimitiveUnitCellVolume>            AUTO </MaxPrimitiveUnitCellVolume>

    <!-- Maximum number of quadruples (q1,q2,q3,q4) taken from selected topographs.-->
    <MaxNumberOfTwoDimTopographs> AUTO </MaxNumberOfTwoDimTopographs>

    <!-- Maximum number of seeds of 3-dimensional topographs -->
    <MaxNumberOfLatticeCandidates> AUTO </MaxNumberOfLatticeCandidates>

    <!--Output for each crystal system? (0:No, 1:Yes)-->
    <OutputTriclinic> 1 </OutputTriclinic>
    <OutputMonoclinicP> 1 </OutputMonoclinicP>
    <OutputMonoclinicB> 1 </OutputMonoclinicB>
    <OutputOrthorhombicP> 1 </OutputOrthorhombicP>
    <OutputOrthorhombicB> 1 </OutputOrthorhombicB>
    <OutputOrthorhombicI> 1 </OutputOrthorhombicI>
    <OutputOrthorhombicF> 1 </OutputOrthorhombicF>
    <OutputTetragonalP> 1 </OutputTetragonalP>
    <OutputTetragonalI> 1 </OutputTetragonalI>
    <OutputRhombohedral> 1 </OutputRhombohedral>
    <OutputHexagonal> 1 </OutputHexagonal>
    <OutputCubicP> 1 </OutputCubicP>
    <OutputCubicI> 1 </OutputCubicI>
    <OutputCubicF> 1 </OutputCubicF>
```

Fig.11-2 Example of *.inp.xml (1/2)

```xml
    <!-- Parameters for output.-->
    <!-- Relative resolution to judge whether two lattices are equivalent or not.
          If the relative difference of two lattice parameters is within this value,
          only that with a better figure of merit is output.-->
    <Resolution> 0.05 </Resolution>

    <!-- Maximum number of false (unindexed) peaks.-->
    <MaxNumberOfUnindexedPeaks> 20 </MaxNumberOfUnindexedPeaks>

    <!-- Number of reflections to calculate figure of merit.-->
    <MaxNumberOfPeaksForFOM> 20 </MaxNumberOfPeaksForFOM>

    <!-- Output the candidates with better FOM than the following value.-->
    <MinFOM> 3 </MinFOM>

    <!-- Number of hkl among input reflections.-->
    <MaxNumberOfMillerIndicesInRange> AUTO </MaxNumberOfMillerIndicesInRange>
    <MinNumberOfMillerIndicesInRange> AUTO </MinNumberOfMillerIndicesInRange>
    <!-- Minimum and maximum of the unit cell edges a, b, c (angstrom).-->
    <MaxUnitCellEdgeABC> 1000 </MaxUnitCellEdgeABC>
    <MinUnitCellEdgeABC> 0 </MinUnitCellEdgeABC>

  </ConographParameters>

  <PeakSearchPSParameters>
    <ParametersForSmoothingDevision>
      <!--NumberOfPointsForSGMethod : odd number.-->
      <NumberOfPointsForSGMethod> 9 </NumberOfPointsForSGMethod>

      <EndOfRegion>
      <!-- The maximum point of smoothing range. -->
        MAX
      </EndOfRegion>
    </ParametersForSmoothingDevision>

    <PeakSearchRange>
      <Begin> 0.0 </Begin>
      <End> MAX </End>
    </PeakSearchRange>

    <!--0 : Use the threshold, 1 : Use a constant times the error of y-value as a threshold.-->
    <UseErrorData> 1 </UseErrorData>

    <!--When "UseErrorData" is 0, it is used as the threshold for peak search.
         Otherwise, "Threshold" times the error of y-value is used as a threshold.-->
    <Threshold> 5.0 </Threshold>

    <!-- 0 : "Threshold" is applied to estimated y-values of peak-tops when the background of the histogram is removed,
          1 : "Threshold" is applied to actual y-values of peak-tops.-->
    <UseBGRemoved> 0 </UseBGRemoved>

    <!-- 0 : deconvolution is not applied.
          1 : deconvolution is applied.-->
    <Alpha2Correction> 0 </Alpha2Correction>
    <Waves>
      <Kalpha1WaveLength> 1.54056 </Kalpha1WaveLength>
      <Kalpha2WaveLength> 1.54439 </Kalpha2WaveLength>
    </Waves>
  </PeakSearchPSParameters>
</ZCodeParameters>
```

Fig. 11-3 Example of *.inp.xml (2/2)

```
IGOR
WAVES/O tof, yint, yerr
BEGIN
     1850.00    2.871904E-001    3.359009E-003
     1854.00    2.834581E-001    3.337111E-003
     1858.00    2.848073E-001    3.351369E-003
～Omitted～
     49564.0    9.989611E-002    1.378697E-002
     49588.0    1.010892E-001    1.386346E-002
END
WAVES/O peak, peakpos, height, FWHM, Flag
BEGIN
       1    3.148311E+003    1.535192E-001    3.749774E+001        1
       2    3.340909E+003    1.676432E-001    2.429063E+001        1
       3    3.697289E+003    1.661457E-001    2.063853E+001        1
～Omitted～
      49    3.133224E+004    2.968128E+000    1.480559E+002        1
      50    4.906641E+004    1.092195E-001    1.791403E+002        1
END
WAVES/O dphase_1, xphase_1, yphase_1, h_1, k_1, l_1
BEGIN
   3.138130E+000    3.133851E+004    0.000000E+000     1     -1     1
   2.717700E+000    2.713443E+004    0.000000E+000     0
   1.921704E+000    1.918059E+004    0.000000E+000     0
～omitted～
   6.405680E-001    6.394727E+003    0.000000E+000     2      2    -8
   6.405680E-001    6.394727E+003    0.000000E+000     0      6    -6
END

X Display yint vs tof
X AppendToGraph yphase_1 vs xphase_1
X ModifyGraph mirror(left)=2
X ModifyGraph mirror(bottom)=2
X ModifyGraph rgb(yint)=(0,65535,65535)
X ModifyGraph
offset(yphase_1)={0,0},mode(yphase_1)=3,marker(yphase_1)=10,msize(yphase_1)=3,mrkThick(ypha
se_1)=0.6,rgb(yphase_1)=(3,52428,1)
```

Only output

Fig. 11-4 Example of *.histogramIgor

```
<ConographOutput>
  <!-- Information on the best M solution for each Bravais type.
            TNB : total number of solutions of the Bravais types,
            M : de Wolff figure of merit,
            Mwu : Wu figure of merit,
            Mrev : reversed de Wolff figure of merit,
            Msym : symmetric de Wolff figure of merit,
            NN : number of lattices in the neighborhood,
            VOL : unit-cell volume.
  Bravais Lattice : TNB, M, Mwu, Mrev, Msym, NN, VOL
            Cubic(F) :         25     7.6120e+000    213     1.5861e+002
            Cubic(I) :         17     2.1801e+000    246     2.0063e+001
            Cubic(P) :          0
          Hexagonal :           4     2.1261e+000     43     1.3385e+001
        Rhombohedral :         20     4.6341e+000    149     1.0755e+002
       Tetragonal(I) :         14     3.3966e+000    633     8.0329e+001
       Tetragonal(P) :          0
  Orthorhombic(F) :             0
  Orthorhombic(I) :             0
  Orthorhombic(B) :             1     2.6029e+000      8     5.7058e+001
  Orthorhombic(P) :             0
     Monoclinic(B) :            0
     Monoclinic(P) :            0
          Triclinic :           0
 -->

 <!-- Information on the selected candidates.-->
 <SelectedLatticeCandidate number="140153">
  <CrystalSystem>          Cubic(F) </CrystalSystem>

  <!-- a, b, c(angstrom), alpha, beta, gamma(deg.)-->
  <LatticeParameters>    5.4354e+000    5.4354e+000    5.4354e+000    9.0000e+001    9.0000e+001    9.0000e+001
</LatticeParamters>

  <!-- A*, B*, C*, D*, E*, F*(angstrom^(-2)).-->
  <ReciprocalLatticeParamters>    3.3848e-002    3.3848e-002    3.3848e-002    0.0000e+000    0.0000e+000
0.0000e+000 </ReciprocalLatticeParamters>
  <!-- A*, B*, C*, D*, E*, F*(angstrom^(-2)) first given by peak-positions.-->
  <InitialReciprocalLatticeParamters>    3.4129e-002    3.4129e-002    3.4129e-002    0.0000e+000    0.0000e+000
0.0000e+000 </InitialReciprocalLatticeParamters>
  <VolumeOfUnitCell>    1.5861e+002 </VolumeOfUnitCell>
  <FigureOfMeritWolff name="Fw20">    7.6120e+000 </FigureOfMeritWolff>
  <NumberOfLatticesInNeighborhood>            213 </NumberOfLatticesInNeighborhood>

  <!-- Number of pairs of hkl and -h-k-l up to the 20th reflection.-->
  <NumberOfMillerIndicesInRange>    2.7750e+001 </NumberOfMillerIndicesInRange>

  <EquivalentLatticeCandidates>
   <LatticeCandidate number="13034">
    <CrystalSystem>          Cubic(I) </CrystalSystem>
    <LatticeParamters>    4.1917e+000    4.1917e+000    4.1917e+000    9.0000e+001    9.0000e+001
9.0000e+001 </LatticeParamters>
    <ReciprocalLatticeParamters>    2.8457e-002    2.8457e-002    5.6913e-002    0.0000e+000    0.0000e+000
0.0000e+000 </ReciprocalLatticeParamters>
    <FigureOfMeritWolff name="Fw20">    1.3537e+000 </FigureOfMeritWolff>
    <NumberOfLatticesInNeighborhood>            213 </NumberOfLatticesInNeighborhood>
   </LatticeCandidate>
～Omitted～
  </EquivalentLatticeCandidates>
```

Fig. 11-5 Example of *.index.xml (1/2)

```
   <IndexingResults>
    <!--          q_obs,          q_cal,          peak_pos,          pos_cal,          closest_hkl,
is_the_difference_between_q_obs_and_q_cal_small_compared_to_q_err?.-->
      4.1501e-002    1.0154e-001    4.9066e+004    3.1339e+004       [-1,1,1]    0
      1.0159e-001    1.0154e-001    3.1332e+004    3.1339e+004      [-1,-1,-1]    1
      2.1784e-001    2.7079e-001    2.1387e+004    1.9181e+004       [0,-2,-2]    0
～Omitted～
      2.2680e+000    2.2678e+000    6.6286e+003    6.6288e+003        [7,3,-3]    1
      2.4367e+000    2.4371e+000    6.3952e+003    6.3947e+003        [-6,6,0]    1
   </IndexingResults>

   <FittingResults>
    <!-- q_obs, q_err, q_cal, peak_pos, peak_width, pos_cal, hkl, fix_or_fit.-->
      4.1501e-002      1.2834e-004      1.0154e-001      4.9066e+004      1.7914e+002
3.1339e+004      [-1,1,1]    0
      1.0159e-001      4.0706e-004      1.0154e-001      3.1332e+004      1.4806e+002
3.1339e+004     [-1,-1,-1]    1
      2.1784e-001      8.7727e-004      2.7079e-001      2.1387e+004      1.0149e+002
1.9181e+004      [0,-2,-2]    0
～omitted～
      2.2680e+000      7.2533e-003      2.2678e+000      6.6286e+003      2.4936e+001
6.6288e+003      [7,3,-3]    1
      2.4367e+000      8.1458e-003      2.4371e+000      6.3952e+003      2.5146e+001
6.3947e+003      [-6,6,0]    1
   </FittingResults>

</SelectedLatticeCandidate>

<!-- Candidates for Cubic(F) -->
～omitted～
</ConographOutput>
```


Fig.11-6 Example of *.index.xml (2/2)

```
<ZCodeParameters>
 <ConographOutput>
  <TypeOfReflectionConditions>
   <Candidates>
    <SpaceGroups> 45(bca),72(bca) </SpaceGroups>
    <ReflectionConditions> hk0:h,k=2n,0kl:k,l=2n </ReflectionConditions>
    <FigureOfMeritWolff name="M20"> 3.126279e+002 </FigureOfMeritWolff>
    <IndexingResults>
     <!-- q_obs, q_err, q_cal, peak_pos, peak_width, pos_cal, hkl, fix_or_fit.-->
  1.016473e-001   9.594352e-004   1.015807e-001   3.132270e+004   1.480559e+002
3.133298e+004          [1,0,-1]       1
  2.708116e-001   2.274422e-003   2.707887e-001   1.917970e+004   8.059404e+001
1.918051e+004          [0,2,0]       1
  3.724714e-001   2.575261e-003   3.724523e-001   1.635279e+004   5.655483e+001
1.635321e+004          [2,1,1]       1
～Omitted～
  2.539049e+000   2.019023e-002   2.539077e+000   6.265138e+003   2.488311e+001
6.265104e+003          [3,4,-5]       1
  2.707958e+000   2.205347e-002   2.707998e+000   6.066813e+003   2.467594e+001
6.066769e+003          [2,6,0]       1
    </IndexingResults>
   </Candidates>

～Omitted～
  </TypeOfReflectionConditions>
 </ConographOutput>
```

Fig. 11-7 Example of *.out.xml

12. Addendum

12.1. Request for citation

Please cite the following when research findings obtained using Conograph are mentioned in academic manuscripts:

R. Oishi-Tomiyasu, ñRobust powder auto-indexing using many peaksò, J. Appl. Cryst., 47 (2014), pp. 593ï 598.

The methods and figures of merit of Conograph are also introduced in the following papers:

- R. Oishi-Tomiyasu, ñA method to enumerate all geometrical ambiguities in powder indexing and its applicationò, submitted.
- R. Oishi-Tomiyasu, ñDistribution rules of systematic absences on the Conway topograph and their application to powder auto-indexingò, Acta Cryst. A69 (2013), pp. 603ï 610.
- R. Oishi-Tomiyasu, ñReversed de Wolff figure of merit and its application to powder indexing solutionsò, J. Appl. Cryst., 46 (2013), pp.1277ï 1282.
- R. Oishi-Tomiyasu, ñRapid Bravais-lattice determination algorithm for lattice parameters containing large observation errorsò, Acta Cryst. A68 (2012), pp. 525ï 535.
- R. Oishi, M. Yonemura, T. Ishigaki, A. Hoshikawa, K. Mori, T. Morishima, S. Torii, T. Kamiyama, ñNew approach to indexing method of powder diffraction patterns using topographsò, Zeitschrift für Kristallographie Supplements 30 (2009), pp. 15ï 20.

12.2. Bug report

Please send the following information to the e-mail address conograph-bug@lists.osdn.me. All comments will be considered and reflected at the time of Conograph version upgrading.

(i) OS used (including 32-bit and 64-bit)
(ii) Conograph version used (indicated in the GUI Help menu)
(iii) Particulars of problem
(iv) Details of conditions when problem occurred
(v) Possibility of recurrence (does it occur always or sometimes?)
(vi) Name, affiliation, e-mail address (to allow us to contact you)

Depending on the contents of the problem, we may request the input/output files and other information. We seek your cooperation in this regard.

References

[1] C. Dong, F. Wu, H. Chen, *Correction of zero shift in powder diffraction patterns using the reflection-pair method*, J. Appl. Cryst., 32, pp. 850ï 853 (1999).

[2] A. D. Mighell, A. Santoro, *Geometrical Ambiguities in the Indexing of Powder Patterns*, J. Appl. Cryst., 8, pp. 372ï 374 (1975).

[3] R. Oishi-Tomiyasu, *A method to enumerate all geometrical ambiguities in powder indexing and its application*, submitted.

[4] R. Oishi-Tomiyasu, *Robust powder auto-indexing using many peaks*, J. Appl. Cryst., 47 (2014), pp. 593ï 598.

[5] R. Oishi-Tomiyasu, *Reversed de Wolff figure of merit and its application to powder indexing solutions*, J. Appl. Cryst., 46 (2013), pp. 1277ï 1282.

[6] P. M. de Wolff, *A simplified criterion for the reliability of a powder pattern indexing*, J. Appl. Cryst., 1, pp. 108ï 113 (1968).

[7] E. Wu, *A modification of the de Wolff figure of merit for reliability of powder pattern indexing*, J. Appl. Cryst., 21, pp. 530ï 535 (1988).